PIConGPU Documentation

Release 0.6.0

The PIConGPU Community

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INSTALLATION

Particle-in-Cell Simulations for the Exascale Era

PIConGPU is a fully relativistic, manycore, 3D3V and 2D3V particle-in-cell (PIC) code. The PIC algorithm is a central tool in plasma physics. It describes the dynamics of a plasma by computing the motion of electrons and ions in the plasma based on the Vlasov-Maxwell system of equations.

Generally, to get started **follow the manual pages in order**. Individual chapters are based on the information in the chapters before. In case you are already fluent in compiling C++ projects and HPC, running PIC simulations or scientific data analysis, feel free to jump the respective sections.

Note: We are migrating our wiki to this manual, but some pages might still be missing. We also have an official homepage .

Note: Are you looking for our latest Doxygen docs for the API?

See http://computationalradiationphysics.github.io/picongpu

CHAPTER

ONE

INSTALLATION

1.1 Introduction

Section author: Axel Huebl

Installing PIConGPU means *installing C++ libraries* that PIConGPU depends on and *setting environment variables* to find those dependencies. The first part is usually the job of a system administrator while the second part needs to be configured on the user side.

Depending on your experience, role, computing environment and expectations for optimal hardware utilization, you have several ways to install and select PIConGPU's dependencies. Choose your favorite *install and environment management method* below, young padawan, and follow the corresponding sections of the next chapters.

1.1.1 Ways to Install

Choose *one* of the installation methods below to get started.

Load Modules

On HPC systems and clusters, software is usually provided by system administrators via a module system (e.g. [modules], [Lmod]). In case our *software dependencies* are available, we usually create a file in our `$HOME` named *<queueName>_picongpu.profile*. It loads according modules and sets *helper environment variables*.

Important: For many HPC systems we have already prepared and maintain an environment which will run out of the box. See if your system is *in the list* so you can skip the installation completely!

Spack

[Spack] is a flexible package manager that can build and organize software dependencies. It can be configured once for your hardware architecture to create optimally tuned binaries and provides modulefile support (e.g. [modules], [Lmod]). Those auto-build modules manage your environment variables and allow easy switching between versions, configurations and compilers.

Build from Source

You choose a supported C++ compiler and configure, compile and install all missing dependencies from source. You are responsible to manage the right versions and configurations. Performance will be ideal if architecture is chosen correctly (and/or if built directly on your hardware). You then set environment variables to find those installs.

Conda

We currently do not have an official conda install (yet). Due to pre-build binaries, performance could be not ideal and HPC cluster support (e.g. MPI) might be very limited. Useful for small desktop or single-node runs.

Nvidia-Docker

Not yet officially supported [nvidia-docker], but we already provide a `Dockerfile` to get started. Performance might be not ideal if the image is not built for the specific local hardware again. Useful for small desktop or single-node runs. We are also working on Singularity images.

1.1.2 References

1.2 Instructions

Section author: Axel Huebl

As explained in the previous section, select and **follow exactly one** of the following install options.

See also:

You will need to understand how to use the terminal.

Warning: Our spack package is still in beta state and is continuously improved. Please feel free to report any issues that you might encounter.

1.2.1 Spack

Section author: Axel Huebl

Preparation

First install spack itself via:

```
# get spack
git clone https://github.com/spack/spack.git $HOME/src/spack

# activate the spack environment
source $HOME/src/spack/share/spack/setup-env.sh

# install a supported compiler
spack compiler list | grep -q gcc@7.3.0 || spack install gcc@7.3.0 && spack load␣
↪gcc@7.3.0 && spack compiler add

# add the PIConGPU repository
git clone https://github.com/ComputationalRadiationPhysics/spack-repo.git $HOME/
↪src/spack-repo

# add the new repo to spack
spack repo add $HOME/src/spack-repo
```

Note: When you open a terminal next time or log back into the machine, make sure to activate the spack environment again via:

```
source $HOME/src/spack/share/spack/setup-env.sh
```

Install

The installation of the latest version of PIConGPU is now as easy as:

```
spack install picongpu %gcc@7.3.0
```

Use PIConGPU

PIConGPU can now be loaded with

```
spack load picongpu
```

For more information on *variants* of the `picongpu` package in spack run `spack info picongpu` and refer to the official spack documentation.

Note: PIConGPU can also run *without a GPU*! For example, to use our OpenMP backend, just add `backend=omp2b` to the two commands above:

```
spack install picongpu backend=omp2b
spack load picongpu backend=omp2b
```

Note: If the install fails or you want to compile for CUDA 9.2, try using GCC 5.5.0:

```
spack compiler list | grep gcc@5.5.0 | spack install gcc@5.5.0 && spack load gcc@5.
↪5.0 && spack compiler add
spack install picongpu %gcc@5.5.0
spack load picongpu %gcc@5.5.0
```

See also:

You will need to understand how to use the terminal.

Warning: Docker images are experimental and not yet fully automated or integrated.

1.2.2 Docker

Section author: Axel Huebl

Preparation

First install nvidia-docker for your distribution. Use version 2 or newer.

Install

The download of a pre-configured image with the latest version of PIConGPU is now as easy as:

```
docker pull ax3l/picongpu
```

Use PIConGPU

Start a pre-configured LWFA live-simulation with

```
docker run --runtime=nvidia -p 2459:2459 -t ax3l/picongpu /bin/bash -lc start_lwfa
# open firefox and isaac client
```

or just open the container and run your own:

```
docker run --runtime=nvidia -it ax3l/picongpu
```

Note: PIConGPU can also run *without a GPU*! We will provide more image variants in the future.

See also:

You will need to understand how to use the terminal.

Note: This section is a short introduction in case you are missing a few software packages, want to try out a cutting edge development version of a software or have no system administrator or software package manager to build and install software for you.

1.2.3 From Source

Section author: Axel Huebl

Don't be afraid, young physicist, self-compiling C/C++ projects is easy, fun and profitable!

Building a project from source essentially requires three steps:

1. configure the project and find its dependencies
2. compile the project
3. install the project

All of the above steps can be performed without administrative rights ("root" or "superuser") as long as the install is not targeted at a system directory (such as `/usr`) but inside a user-writable directory (such as `$HOME` or a project directory).

Preparation

In order to compile projects from source, we assume you have individual directories created to store *source code*, *build temporary files* and *install* the projects to:

```
# source code
mkdir $HOME/src
# temporary build directory
mkdir $HOME/build
# install target for dependencies
mkdir $HOME/lib
```

Note that on some supercomputing systems, you might need to install the final software outside of your home to make dependencies available during run-time (when the simulation runs). Use a different path for the last directory then.

What is Compiling?

Note: This section is **not** yet the installation of PIConGPU from source. It just introduces in general how one compiles projects.

If you like to skip this introduction, *jump straight to the dependency install section*.

Compling can differ in two principle ways: building *inside* the source directory ("in-source") and in a *temporary directory* ("out-of-source"). Modern projects prefer the latter and use a build system such as [CMake].

An example could look like this

```
# go to an empty, temporary build directory
cd $HOME/build
rm -rf ../build/*

# configurate, build and install into $HOME/lib/project
cmake -DCMAKE_INSTALL_PREFIX=$HOME/lib/project $HOME/src/project_to_compile
make
make install
```

Often, you want to pass further options to CMake with `-DOPTION=VALUE` or modify them interactively with `ccmake .` after running the initial cmake command. The second step which compiles the project can in many cases be parallelized by `make -j`. In the final install step, you might need to prefix it with `sudo` in case `CMAKE_INSTALL_PREFIX` is pointing to a system directory.

Some older projects often build *in-source* and use a build system called *autotools*. The syntax is still very similar:

```
# go to the source directory of the project
cd $HOME/src/project_to_compile

# configurate, build and install into $HOME/lib/project
configure --prefix=$HOME/lib/project
make
make install
```

One can usually pass further options with `--with-something=VALUE` or `--enable-thing` to `configure`. See `configure --help` when installing an *autotools* project.

That is all on the theory of building projects from source!

Now Start

You now know all the basics to install from source. Continue with the following section to *build our dependencies*.

References

If anything goes wrong, an overview of the full list of PIConGPU dependencies is provided in *section Dependencies*.

After installing, the last step is the setup of a *profile*.

See also:

You will need to understand how to use the terminal, what are environment variables and please read our *compiling introduction*.

Note: If you are a scientific user at a supercomputing facility we might have already prepared a software setup for you. See the *following chapter* if you can skip this step fully or in part by loading existing modules on those

systems.

1.3 Dependencies

Section author: Axel Huebl

1.3.1 Overview

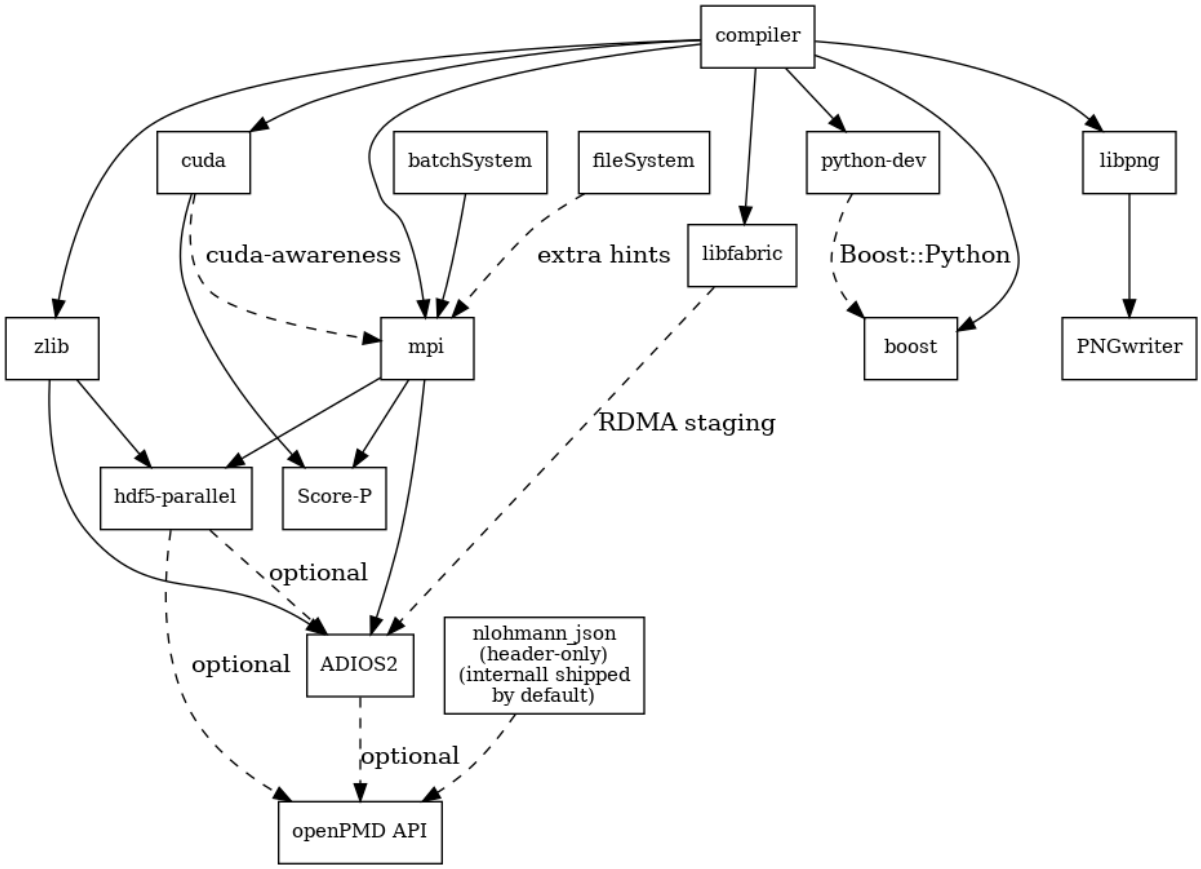

Fig. 1.1: Overview of inter-library dependencies for parallel execution of PIConGPU on a typical HPC system. Due to common binary incompatibilities between compilers, MPI and boost versions, we recommend to organize software with a version-aware package manager such as spack and to deploy a hierarchical module system such as lmod. An Lmod example setup can be found here.

1.3.2 Requirements

Mandatory

gcc

- 5.5 - 10.0 (if you want to build for Nvidia GPUs, supported compilers depend on your current CUDA version)
  - CUDA 9.2 - 10.0: Use gcc 5.5 - 7
  - CUDA 10.1/10.2: Use gcc 5.5 - 8

  - CUDA 11.x: Used gcc 5.5 - 10.0
- *note:* be sure to build all libraries/dependencies with the *same* gcc version; GCC 5 or newer is recommended
- *Debian/Ubuntu:*
  - `sudo apt-get install gcc-5 g++-5 build-essential`
  - `sudo update-alternatives --install /usr/bin/gcc gcc /usr/bin/gcc-5 60 --slave /usr/bin/g++ g++ /usr/bin/g++-5`
- *Arch Linux:*
  - `sudo pacman --sync base-devel`
  - if the installed version of **gcc** is too new, compile an older gcc
- *Spack:*
  - `spack install gcc@5.5.0`
  - make it the default in your packages.yaml or *suffix* all following `spack install` commands with a *space* and `%gcc@5.5.0`

CMake

- 3.15.0 or higher
- *Debian/Ubuntu:* `sudo apt-get install cmake file cmake-curses-gui`
- *Arch Linux:* `sudo pacman --sync cmake`
- *Spack:* `spack install cmake`

MPI 2.3+

- **OpenMPI** 1.7+ / **MVAPICH2** 1.8+ or similar
- for running on Nvidia GPUs, perform a GPU aware MPI install *after* installing CUDA
- *Debian/Ubuntu:* `sudo apt-get install libopenmpi-dev`
- *Arch Linux:* `sudo pacman --sync openmpi`
- *Spack:*
  - *GPU support:* `spack install openmpi+cuda`
  - *CPU only:* `spack install openmpi`
- *environment:*
  - `export MPI_ROOT=<MPI_INSTALL>`
  - as long as CUDA awareness (`openmpi+cuda`) is missing: `export OMPI_MCA_mpi_leave_pinned=0`

zlib

- *Debian/Ubuntu:* `sudo apt-get install zlib1g-dev`
- *Arch Linux:* `sudo pacman --sync zlib`
- *Spack:* `spack install zlib`
- *from source:*
  - `./configure --prefix=$HOME/lib/zlib`

  - `make && make install`

- *environent:* (assumes install from source in `$HOME/lib/zlib`)
  - `export ZLIB_ROOT=$HOME/lib/zlib`
  - `export LD_LIBRARY_PATH=$ZLIB_ROOT/lib:$LD_LIBRARY_PATH`
  - `export CMAKE_PREFIX_PATH=$ZLIB_ROOT:$CMAKE_PREFIX_PATH`

boost

- 1.65.1 - 1.74.0 (`program_options`, `filesystem`, `system`, `math`, `serialization` and header-only libs, optional: `fiber` with `context`, `thread`, `chrono`, `atomic`, `date_time`)
- *Debian/Ubuntu:* `sudo apt-get install libboost-program-options-dev libboost-filesystem-dev libboost-system-dev libboost-thread-dev libboost-chrono-dev libboost-atomic-dev libboost-date-time-dev libboost-math-dev libboost-serialization-dev libboost-fiber-dev libboost-context-dev`
- *Arch Linux:* `sudo pacman --sync boost`
- *Spack:* `spack install boost`
- *from source:*
  - `curl -Lo boost_1_65_1.tar.gz https://dl.bintray.com/boostorg/release/1.65.1/source/boost_1_65_1.tar.gz`
  - `tar -xzf boost_1_65_1.tar.gz`
  - `cd boost_1_65_1`
  - `./bootstrap.sh --with-libraries=atomic,chrono,context,date_time,fiber,filesystem,math,program_options,serialization,system,thread --prefix=$HOME/lib/boost`
  - `./b2 cxxflags="-std=c++11" -j4 && ./b2 install`
- *environment:* (assumes install from source in `$HOME/lib/boost`)
  - `export BOOST_ROOT=$HOME/lib/boost`
  - `export LD_LIBRARY_PATH=$BOOST_ROOT/lib:$LD_LIBRARY_PATH`

git

- 1.7.9.5 or higher
- *Debian/Ubuntu:* `sudo apt-get install git`
- *Arch Linux:* `sudo pacman --sync git`
- *Spack:* `spack install git`

rsync

- *Debian/Ubuntu:* `sudo apt-get install rsync`
- *Arch Linux:* `sudo pacman --sync rsync`
- *Spack:* `spack install rsync`

alpaka 0.6.X

- alpaka is included in the PIConGPU source code

cupla 0.3.0

- cupla is included in the PIConGPU source code

mallocMC 2.6.0crp-dev

- only required for CUDA backend
- mallocMC is included in the PIConGPU source code

PIConGPU Source Code

- `git clone https://github.com/ComputationalRadiationPhysics/picongpu.git $HOME/src/picongpu`
  - *optional:* update the source code with `cd $HOME/src/picongpu && git fetch && git pull`
  - *optional:* change to a different branch with `git branch` (show) and `git checkout <BranchName>` (switch)
- *environment*:
  - `export PICSRC=$PICHOME/src/picongpu`
  - `export PIC_EXAMPLES=$PICSRC/share/picongpu/examples`
  - `export PATH=$PICSRC:$PATH`
  - `export PATH=$PICSRC/bin:$PATH`
  - `export PATH=$PICSRC/src/tools/bin:$PATH`
  - `export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH`

Optional Libraries

CUDA

- 9.2 - 10.2
- required if you want to run on Nvidia GPUs
- *Debian/Ubuntu:* `sudo apt-get install nvidia-cuda-toolkit`
- *Arch Linux:* `sudo pacman --sync cuda`
- *Spack:* `spack install cuda`
- at least one **CUDA** capable **GPU**
- *compute capability*: `sm_30` or higher
- full list of CUDA GPUs and their *compute capability*
- More is always better. Especially, if we are talking GPUs :-)
- *environment:*
  - `export CUDA_ROOT=<CUDA_INSTALL>`

If you do not install the following libraries, you will not have the full amount of PIConGPU plugins. We recommend to install at least **pngwriter** and **openPMD**.

libpng

- 1.2.9+ (requires *zlib*)
- *Debian/Ubuntu dependencies:* `sudo apt-get install libpng-dev`
- *Arch Linux dependencies:* `sudo pacman --sync libpng`
- *Spack:* `spack install libpng`
- *from source:*
  - `mkdir -p ~/src ~/lib`
  - `cd ~/src`
  - `curl -Lo libpng-1.6.34.tar.gz ftp://ftp-osl.osuosl.org/pub/libpng/src/libpng16/libpng-1.6.34.tar.gz`
  - `tar -xf libpng-1.6.34.tar.gz`
  - `cd libpng-1.6.34`
  - `CPPFLAGS=-I$HOME/lib/zlib/include LDFLAGS=-L$HOME/lib/zlib/lib ./configure --enable-static --enable-shared --prefix=$HOME/lib/libpng`
  - `make`
  - `make install`
- *environment:* (assumes install from source in `$HOME/lib/libpng`)
  - `export PNG_ROOT=$HOME/lib/libpng`
  - `export CMAKE_PREFIX_PATH=$PNG_ROOT:$CMAKE_PREFIX_PATH`
  - `export LD_LIBRARY_PATH=$PNG_ROOT/lib:$LD_LIBRARY_PATH`

pngwriter

- 0.7.0+ (requires *libpng*, *zlib*, and optional *freetype*)
- *Spack:* `spack install pngwriter`
- *from source:*
  - `mkdir -p ~/src ~/build ~/lib`
  - `git clone https://github.com/pngwriter/pngwriter.git ~/src/pngwriter/`
  - `cd ~/build`
  - `cmake -DCMAKE_INSTALL_PREFIX=$HOME/lib/pngwriter ~/src/pngwriter`
  - `make install`
- *environment:* (assumes install from source in `$HOME/lib/pngwriter`)
  - `export CMAKE_PREFIX_PATH=$HOME/lib/pngwriter:$CMAKE_PREFIX_PATH`
  - `export LD_LIBRARY_PATH=$HOME/lib/pngwriter/lib:$LD_LIBRARY_PATH`

HDF5

- 1.8.13+
- standard shared version (no C++, enable parallel)
- *Debian/Ubuntu:* `sudo apt-get install libhdf5-openmpi-dev`
- *Arch Linux:* `sudo pacman --sync hdf5-openmpi`
- *Spack:* `spack install hdf5~fortran`
- *from source:*
  - `mkdir -p ~/src ~/lib`
  - `cd ~/src`
  - download hdf5 source code from release list of the HDF5 group, for example:
  - `curl -Lo hdf5-1.8.20.tar.gz https://support.hdfgroup.org/ftp/HDF5/releases/hdf5-1.8/hdf5-1.8.20/src/hdf5-1.8.20.tar.gz`
  - `tar -xzf hdf5-1.8.20.tar.gz`
  - `cd hdf5-1.8.20`
  - `./configure --enable-parallel --enable-shared --prefix $HOME/lib/hdf5/`
  - `make`
  - *optional:* `make test`
  - `make install`
  - If you encounter errors related to linking MPI during `./configure`, you might try setting the compiler manually via `./configure --enable-parallel --enable-shared --prefix $HOME/lib/hdf5/ CC=mpicc CXX=mpic++`.
- *environment:* (assumes install from source in `$HOME/lib/hdf5`)
  - `export HDF5_ROOT=$HOME/lib/hdf5`
  - `export LD_LIBRARY_PATH=$HDF5_ROOT/lib:$LD_LIBRARY_PATH`

c-blosc

- general purpose compressor, used in ADIOS2 for in situ data reduction
- *Debian/Ubuntu:* `sudo apt-get install libblosc-dev`
- *Arch Linux:* `sudo pacman --sync blosc`
- *Spack:* `spack install c-blosc`
- *from source:*
  - `mkdir -p ~/src ~/build ~/lib`
  - `cd ~/src`
  - `curl -Lo c-blosc-1.15.0.tar.gz https://github.com/Blosc/c-blosc/archive/v1.15.0.tar.gz`
  - `tar -xzf c-blosc-1.15.0.tar.gz`
  - `cd ~/build && rm -rf ../build/*`
  - `cmake -DCMAKE_INSTALL_PREFIX=$HOME/lib/c-blosc -DPREFER_EXTERNAL_ZLIB=ON ~/src/c-blosc-1.15.0/`

  - `make`
  - `make install`
- *environment:* (assumes install from source in `$HOME/lib/c-blosc`)
  - `export BLOSC_ROOT=$HOME/lib/c-blosc`
  - `export CMAKE_PREFIX_PATH=$BLOSC_ROOT:$CMAKE_PREFIX_PATH`
  - `export LD_LIBRARY_PATH=$BLOSC_ROOT/lib:$LD_LIBRARY_PATH`

openPMD API

- 0.12.0+ (bare minimum) / 0.13.0+ (for streaming IO)
- *Spack*: `spack install openpmd-api`
- For usage in PIConGPU, the openPMD API must have been built either with support for ADIOS2 or HDF5 (or both). When building the openPMD API from source (described below), these dependencies must be built and installed first.
  - For ADIOS2, CMake build instructions can be found in the official documentation. The default configuration should generally be sufficient, the `CMAKE_INSTALL_PREFIX` should be set to a fitting location.
  - For HDF5, CMake build instructions can be found in the official documentation. The parameters `-DHDF5_BUILD_CPP_LIB=OFF -DHDF5_ENABLE_PARALLEL=ON` are required, the `CMAKE_INSTALL_PREFIX` should be set to a fitting location.
- *from source:*
  - `mkdir -p ~/src ~/lib`
  - `cd ~/src`
  - `git clone https://github.com/openPMD/openPMD-api.git`
  - `cd openPMD-api`
  - `mkdir build && cd build`
  - `cmake .. -DopenPMD_USE_MPI=ON -DCMAKE_INSTALL_PREFIX=~/lib/openPMD-api` Optionally, specify the parameters `-DopenPMD_USE_ADIOS2=ON -DopenPMD_USE_HDF5=ON`. Otherwise, these parameters are set to `ON` automatically if CMake detects the dependencies on your system.
  - `make -j $(nproc) install`
- environment:* (assumes install from source in `$HOME/lib/openPMD-api`)
  - `export CMAKE_PREFIX_PATH="$HOME/lib/openPMD-api:$CMAKE_PREFIX_PATH"`
  - `export LD_LIBRARY_PATH="$HOME/lib/openPMD-api/lib:$LD_LIBRARY_PATH"`
- If PIConGPU is built with openPMD output enabled, the JSON library nlohmann_json will automatically be used, found in the `thirdParty/` directory. By setting the CMake parameter `PIC_nlohmann_json_PROVIDER=extern`, CMake can be instructed to search for an installation of nlohmann_json externally. Refer to LICENSE.md for further information.

ISAAC

- 1.4.0+
- requires *boost* (header only), *IceT*, *Jansson*, *libjpeg* (preferably *libjpeg-turbo*), *libwebsockets* (only for the ISAAC server, but not the plugin itself)
- enables live in situ visualization, see more here Plugin description

- *Spack:* `spack install isaac`
- *from source:* build the *in situ library* and its dependencies as described in ISAAC's INSTALL.md
- *environment:* set environment variable `CMAKE_PREFIX_PATH` for each dependency and the ISAAC in situ library

VampirTrace

- for developers: performance tracing support
- download 5.14.4 or higher, e.g. from www.tu-dresden.de
- *from source:*
  - `mkdir -p ~/src ~/build ~/lib`
  - `cd ~/src`
  - `curl -Lo VampirTrace-5.14.4.tar.gz "http://wwwpub.zih.tu-dresden.de/~mlieber/dcount/dcount.php?package=vampirtrace&get=VampirTrace-5.14.4.tar.gz"`
  - `tar -xzf VampirTrace-5.14.4.tar.gz`
  - `cd VampirTrace-5.14.4`
  - `./configure --prefix=$HOME/lib/vampirtrace --with-cuda-dir=<CUDA_ROOT>`
  - `make all -j`
  - `make install`
- *environment:* (assumes install from source in `$HOME/lib/vampirtrace`)
  - `export VT_ROOT=$HOME/lib/vampirtrace`
  - `export PATH=$VT_ROOT/bin:$PATH`

See also:

You need to have all *dependencies installed* to complete this chapter.

1.4 picongpu.profile

Section author: Axel Huebl

Use a `picongpu.profile` file to set up your software environment without colliding with other software. Ideally, store that file directly in your `$HOME/` and source it after connecting to the machine:

```
source $HOME/picongpu.profile
```

We listed some example `picongpu.profile` files below which can be used to set up PIConGPU's dependencies on various HPC systems.

1.4.1 Hemera (HZDR)

System overview: link (internal)

User guide: *None*

Production directory: `/bigdata/hplsim/` with `external/`, `scratch/`, `development/` and `production/`

For this profile to work, you need to download the *PIConGPU source code* manually.

Queue: defq (2x Intel Xeon Gold 6148, 20 Cores + 20 HyperThreads/CPU)

```
# Name and Path of this Script ################################# (DO NOT change!)
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ################################# (edit the following lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on batch system jobs: NONE, BEGIN, END, FAIL, REQUEUE, ALL,
#     TIME_LIMIT, TIME_LIMIT_90, TIME_LIMIT_80 and/or TIME_LIMIT_50
export MY_MAILNOTIFY="NONE"
export MY_MAIL="someone@example.com"
export MY_NAME="$(whoami) <$MY_MAIL>"

# Text Editor for Tools ######################################## (edit this line)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
#export EDITOR="nano"

# General modules ###############################################################
#
module purge
module load git
module load gcc/7.3.0
module load cmake/3.15.2
module load openmpi/4.0.4-csk
module load boost/1.68.0

# Other Software ################################################################
#
module load zlib/1.2.11
module load c-blosc/1.14.4

module load hdf5-parallel/1.10.5
module load python/3.6.5
module load libfabric/1.11.1
module load adios2/2.7.1
module load openpmd/0.13.2

module load libpng/1.6.35
module load pngwriter/0.7.0

# Environment ###################################################################
#
#export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$BOOST_LIB

export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="omp2b:skylake-avx512"

export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

# "tbg" default options ########################################################
#   - SLURM (sbatch)
#   - "defq" queue
export TBG_SUBMIT="sbatch"
export TBG_TPLFILE="etc/picongpu/hemera-hzdr/defq.tpl"
# use defq for regular queue and defq_low for low priority queue
export TBG_partition="defq"
```

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```
# allocate an interactive shell for one hour
#   getNode 2  # allocates two interactive nodes (default: 1)
function getNode() {
    if [ -z "$1" ] ; then
        numNodes=1
    else
        numNodes=$1
    fi
    srun --time=1:00:00 --nodes=$numNodes --ntasks-per-node=2 --cpus-per-task=20  -
↪-mem=360000 -p defq --pty bash
}

# allocate an interactive shell for one hour
#   getDevice 2  # allocates two interactive devices (default: 1)
function getDevice() {
    if [ -z "$1" ] ; then
        numDevices=1
    else
        if [ "$1" -gt 2 ] ; then
            echo "The maximal number of devices per node is 2." 1>&2
            return 1
        else
            numDevices=$1
        fi
    fi
    srun --time=1:00:00 --ntasks-per-node=$(($numDevices)) --cpus-per-task=$((20 *
↪$numDevices)) --mem=$((180000 * numDevices)) -p defq --pty bash
}

# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

Queue: gpu (4x NVIDIA P100 16GB)

```
# Name and Path of this Script ################################ (DO NOT change!)
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ################################# (edit the following lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on batch system jobs: NONE, BEGIN, END, FAIL, REQUEUE, ALL,
#     TIME_LIMIT, TIME_LIMIT_90, TIME_LIMIT_80 and/or TIME_LIMIT_50
export MY_MAILNOTIFY="NONE"
export MY_MAIL="someone@example.com"
export MY_NAME="$(whoami) <$MY_MAIL>"

# Text Editor for Tools ########################################## (edit this line)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
#export EDITOR="nano"

# General modules ###############################################################
#
module purge
module load git
module load gcc/7.3.0
```

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```
module load cmake/3.15.2
module load cuda/11.2
module load openmpi/4.0.4-cuda112
module load boost/1.68.0

# Other Software ##############################################################
#
module load zlib/1.2.11
module load c-blosc/1.14.4

module load hdf5-parallel/1.12.0-cuda112
module load python/3.6.5
module load libfabric/1.11.1-co79
module load adios2/2.7.1-cuda112
module load openpmd/0.13.2-cuda112-adios271

module load libpng/1.6.35
module load pngwriter/0.7.0

# Environment #################################################################
#
#export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$BOOST_LIB

export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="cuda:60"

export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

# "tbg" default options ########################################################
#   - SLURM (sbatch)
#   - "gpu" queue
export TBG_SUBMIT="sbatch"
export TBG_TPLFILE="etc/picongpu/hemera-hzdr/gpu.tpl"
# use gpu for regular queue and gpu_low for low priority queue
export TBG_partition="gpu"


# allocate an interactive shell for one hour
#   getNode 2  # allocates two interactive nodes (default: 1)
function getNode() {
    if [ -z "$1" ] ; then
        numNodes=1
    else
        numNodes=$1
    fi
    srun  --time=1:00:00 --nodes=$numNodes --ntasks-per-node=4 --cpus-per-task=6 --
↪gres=gpu:4 --mem=378000 -p gpu --pty bash
}

# allocate an interactive shell for one hour
#   getDevice 2  # allocates two interactive devices (default: 1)
function getDevice() {
    if [ -z "$1" ] ; then
        numGPUs=1
    else
        if [ "$1" -gt 4 ] ; then
```

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```
            echo "The maximal number of devices per node is 4." 1>&2
            return 1
        else
            numGPUs=$1
        fi
    fi
    srun  --time=1:00:00 --ntasks-per-node=$(($numGPUs)) --cpus-per-task=6 --
↪gres=gpu:$numGPUs --mem=$((94500 * numGPUs)) -p gpu --pty bash
}

# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

Queue: fwkt_v100 (4x NVIDIA V100 32GB)

```
# Name and Path of this Script ################################# (DO NOT change!)
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ################################# (edit the following lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on batch system jobs: NONE, BEGIN, END, FAIL, REQUEUE, ALL,
#     TIME_LIMIT, TIME_LIMIT_90, TIME_LIMIT_80 and/or TIME_LIMIT_50
export MY_MAILNOTIFY="NONE"
export MY_MAIL="someone@example.com"
export MY_NAME="$(whoami) <$MY_MAIL>"

# Text Editor for Tools ######################################## (edit this line)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
#export EDITOR="nano"

# General modules ###############################################################
#
module purge
module load git
module load gcc/7.3.0
module load cmake/3.15.2
module load cuda/11.2
module load openmpi/4.0.4-cuda112
module load boost/1.68.0

# Other Software ################################################################
#
module load zlib/1.2.11
module load c-blosc/1.14.4

module load hdf5-parallel/1.12.0-cuda112
module load python/3.6.5
module load libfabric/1.11.1-co79
module load adios2/2.7.1-cuda112
module load openpmd/0.13.2-cuda112-adios271

module load libpng/1.6.35
module load pngwriter/0.7.0
```

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```
# Environment ##################################################################
#
#export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$BOOST_LIB

export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="cuda:70"

export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

# "tbg" default options ########################################################
#   - SLURM (sbatch)
#   - "fwkt_v100" queue
export TBG_SUBMIT="sbatch"
export TBG_TPLFILE="etc/picongpu/hemera-hzdr/fwkt_v100.tpl"
# use fwkt_v100 for regular queue and casus_low for low priority queue
export TBG_partition="fwkt_v100"

# allocate an interactive shell for one hour
#   getNode 2  # allocates two interactive nodes (default: 1)
function getNode() {
    if [ -z "$1" ] ; then
        numNodes=1
    else
        numNodes=$1
    fi
    srun  --time=1:00:00 --nodes=$numNodes --ntasks-per-node=4 --cpus-per-task=6 --
↪gres=gpu:4 --mem=378000 -p fwkt_v100 -A fwkt_v100 --pty bash
}

# allocate an interactive shell for one hour
#   getDevice 2  # allocates two interactive devices (default: 1)
function getDevice() {
    if [ -z "$1" ] ; then
        numGPUs=1
    else
        if [ "$1" -gt 4 ] ; then
            echo "The maximal number of devices per node is 4." 1>&2
            return 1
        else
            numGPUs=$1
        fi
    fi
    srun  --time=1:00:00 --ntasks-per-node=$(($numGPUs)) --cpus-per-task=6 --
↪gres=gpu:$numGPUs --mem=$((94500 * numGPUs)) -p fwkt_v100 -A fwkt_v100 --pty bash
}

# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

Queue: k20 (4x Nvidia K20m GPUs 4.7GB)

```
# Name and Path of this Script ################################ (DO NOT change!)
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ################################# (edit the following lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on batch system jobs: NONE, BEGIN, END, FAIL, REQUEUE, ALL,
#     TIME_LIMIT, TIME_LIMIT_90, TIME_LIMIT_80 and/or TIME_LIMIT_50
export MY_MAILNOTIFY="NONE"
export MY_MAIL="someone@example.com"
export MY_NAME="$(whoami) <$MY_MAIL>"

# Text Editor for Tools ####################################### (edit this line)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
#export EDITOR="nano"

# General modules ##############################################################
#
module purge
module load git
module load gcc/7.3.0
module load cmake/3.15.2
module load cuda/11.2
module load openmpi/4.0.4-cuda112
module load boost/1.68.0

# Other Software ###############################################################
#
module load zlib/1.2.11
module load c-blosc/1.14.4

module load hdf5-parallel/1.12.0-cuda112
module load python/3.6.5
module load libfabric/1.11.1-co79
module load adios2/2.7.1-cuda112
module load openpmd/0.13.2-cuda112-adios271

module load libpng/1.6.35
module load pngwriter/0.7.0

# Environment ##################################################################
#
#export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$BOOST_LIB

export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="cuda:35"

export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

# "tbg" default options ########################################################
#   - SLURM (sbatch)
#   - "k20" queue
export TBG_SUBMIT="sbatch"
export TBG_TPLFILE="etc/picongpu/hemera-hzdr/k20.tpl"
# use k20 for regular queue and k20_low for low priority queue
export TBG_partition="k20"
```

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```
# allocate an interactive shell for one hour
#   getNode 2  # allocates two interactive nodes (default: 1)
function getNode() {
    if [ -z "$1" ] ; then
        numNodes=1
    else
        numNodes=$1
    fi
    srun  --time=1:00:00 --nodes=$numNodes --ntasks-per-node=4 --cpus-per-task=2 --
↪gres=gpu:4 -A k20 --mem=62000 -p k20 --pty bash
}

# allocate an interactive shell for one hour
#   getDevice 2  # allocates two interactive devices (default: 1)
function getDevice() {
    if [ -z "$1" ] ; then
        numGPUs=1
    else
        if [ "$1" -gt 4 ] ; then
            echo "The maximal number of devices per node is 4." 1>&2
            return 1
        else
            numGPUs=$1
        fi
    fi
    srun  --time=1:00:00 --ntasks-per-node=$(($numGPUs)) --cpus-per-task=2 --
↪gres=gpu:$numGPUs -A k20 --mem=$((15500 * numGPUs)) -p k20 --pty bash
}

# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

Queue: k80 (8x NVIDIA K80 12GB)

```
# Name and Path of this Script ################################ (DO NOT change!)
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ################################# (edit the following lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on batch system jobs: NONE, BEGIN, END, FAIL, REQUEUE, ALL,
#     TIME_LIMIT, TIME_LIMIT_90, TIME_LIMIT_80 and/or TIME_LIMIT_50
export MY_MAILNOTIFY="NONE"
export MY_MAIL="someone@example.com"
export MY_NAME="$(whoami) <$MY_MAIL>"

# Text Editor for Tools ########################################## (edit this line)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
#export EDITOR="nano"

# General modules ###############################################################
#
module purge
```

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```
module load git
module load gcc/7.3.0
module load cmake/3.15.2
module load cuda/11.2
module load openmpi/4.0.4-cuda112
module load boost/1.68.0

# Other Software ##############################################################
#
module load zlib/1.2.11
module load c-blosc/1.14.4

module load hdf5-parallel/1.12.0-cuda112
module load python/3.6.5
module load libfabric/1.11.1-co79
module load adios2/2.7.1-cuda112
module load openpmd/0.13.2-cuda112-adios271

module load libpng/1.6.35
module load pngwriter/0.7.0

# Environment #################################################################
#
#export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$BOOST_LIB

export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="cuda:37"

export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

# "tbg" default options ########################################################
#   - SLURM (sbatch)
#   - "k80" queue
export TBG_SUBMIT="sbatch"
export TBG_TPLFILE="etc/picongpu/hemera-hzdr/k80.tpl"
# use k80 for regular queue and k80_low for low priority queue
export TBG_partition="k80"


# allocate an interactive shell for one hour
#   getNode 2  # allocates two interactive nodes (default: 1)
function getNode() {
    if [ -z "$1" ] ; then
        numNodes=1
    else
        numNodes=$1
    fi
    srun  --time=1:00:00 --nodes=$numNodes --ntasks-per-node=8 --cpus-per-task=2 --
↪gres=gpu:8 -A k80 --mem=238000 -p k80 --pty bash
}

# allocate an interactive shell for one hour
#   getDevice 2  # allocates two interactive devices (default: 1)
function getDevice() {
    if [ -z "$1" ] ; then
        numGPUs=1
```

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```
    else
        if [ "$1" -gt 8 ] ; then
            echo "The maximal number of devices per node is 8." 1>&2
            return 1
        else
            numGPUs=$1
        fi
    fi
    srun  --time=1:00:00 --ntasks-per-node=$(($numGPUs)) --cpus-per-task=2 --
↪gres=gpu:$numGPUs -A k80 --mem=$((29750 * numGPUs)) -p k80 --pty bash
}

# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

1.4.2 Summit (ORNL)

System overview: link

User guide: link

Production directory: usually `$PROJWORK/$proj/` (link). Note that `$HOME` is mounted on compute nodes as read-only.

For this profile to work, you need to download the *PIConGPU source code* and install *PNGwriter* manually.

V100 GPUs (recommended)

```
# Name and Path of this Script ################################ (DO NOT change!)
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ################################ (edit the following lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on job (-B)egin, Fi(-N)ish
export MY_MAILNOTIFY=""
export MY_MAIL="someone@example.com"
export MY_NAME="$(whoami) <$MY_MAIL>"

# Project Information ######################################### (edit this line)
#   - project account for computing time
export proj=<yourProject>

# Text Editor for Tools ####################################### (edit this line)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
#module load nano
#export EDITOR="nano"

# basic environment ###########################################################
module load gcc/6.4.0  e4s/21.02  spectrum-mpi/10.3.1.2-20200121

export CC=$(which gcc)
export CXX=$(which g++)

# required tools and libs
```

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```
module load git/2.29.0
module load cmake/3.20.2
module load cuda/10.2.89
module load boost/1.66.0

# plugins (optional) ##################################################################
module load hdf5/1.10.7
module load c-blosc/1.21.0 zfp/0.5.5 sz/2.1.11.1 lz4/1.9.3
module load adios2/2.7.1
module load openpmd-api/0.13.2

#export T3PIO_ROOT=$PROJWORK/$proj/lib/t3pio
#export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$T3PIO_ROOT/lib

module load zlib/1.2.11
module load libpng/1.6.37 freetype/2.9.1
# optionally install pngwriter yourself:
#   https://github.com/pngwriter/pngwriter#install
# export PNGwriter_ROOT=<your pngwriter install directory>  # e.g., ${HOME}/sw/
↪pngwriter
# export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$PNGwriter_ROOT/lib

# helper variables and tools ##########################################################
export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="cuda:70"

export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

# fix MPI collectives by disabling IBM's optimized barriers
# https://github.com/ComputationalRadiationPhysics/picongpu/issues/3814
export OMPI_MCA_coll_ibm_skip_barrier=true

alias getNode="bsub -P $proj -W 2:00 -nnodes 1 -Is /bin/bash"

# "tbg" default options ###############################################################
export TBG_SUBMIT="bsub"
export TBG_TPLFILE="etc/picongpu/summit-ornl/gpu_batch.tpl"

# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

1.4.3 Piz Daint (CSCS)

System overview: link

User guide: link

Production directory: `$SCRATCH` (link).

For this profile to work, you need to download the *PIConGPU source code* and install *boost, zlib, libpng, c-blosc, PNGwriter and ADIOS* manually.

Note: The MPI libraries are lacking Fortran bindings (which we do not need anyway). During the install of ADIOS, make sure to add to `configure` the `--disable-fortran` flag.

Note: Please find a Piz Daint quick start from August 2018 here.

```
# Name and Path of this Script ################################ (DO NOT change!)
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ################################ (edit the following lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on batch system jobs: NONE, BEGIN, END, FAIL, REQUEUE, ALL,
#     TIME_LIMIT, TIME_LIMIT_90, TIME_LIMIT_80 and/or TIME_LIMIT_50
export MY_MAILNOTIFY="NONE"
export MY_MAIL="someone@example.com"
export MY_NAME="$(whoami) <$MY_MAIL>"

# Text Editor for Tools ################################ (edit those lines)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
# module load nano
#export EDITOR="nano"

# Programming Environment ##################################################
#
# if the wrong environment is loaded we switch to the gnu environment
# note: this loads gcc/5.3.0 (6.0.4 is the version of the programming env!)
CRAYENV_FOUND=$(module li 2>&1 | grep "PrgEnv-cray" > /dev/null && { echo 0; } ||
↪{ echo 1; })
if [ $CRAYENV_FOUND -eq 0 ]; then
    module swap PrgEnv-cray PrgEnv-gnu/6.0.4
else
    module load PrgEnv-gnu/6.0.4
fi

module load daint-gpu
# currently loads CUDA 8.0
module load craype-accel-nvidia60

# Compile for cluster nodes
#   (CMake likes to unwrap the Cray wrappers)
export CC=$(which cc)
export CXX=$(which CC)

# define cray compiler target architecture
# if not defined the linker crashed because wrong from */lib instead
# of */lib64 are used
export CRAY_CPU_TARGET=x86-64

# Libraries ################################################################
module load CMake/3.15.0

module load cray-mpich/7.6.0
module load cray-hdf5-parallel/1.10.0.3

# Self-Build Software ######################################################
#
# needs to be compiled by the user
export PIC_LIBS="$HOME/lib"
export BOOST_ROOT=$PIC_LIBS/boost-1.65.1
```

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```
export ZLIB_ROOT=$PIC_LIBS/zlib-1.2.11
export PNG_ROOT=$PIC_LIBS/libpng-1.6.34
export BLOSC_ROOT=$PIC_LIBS/blosc-1.12.1
export PNGwriter_DIR=$PIC_LIBS/pngwriter-0.7.0

export LD_LIBRARY_PATH=$BOOST_ROOT/lib:$LD_LIBRARY_PATH
export LD_LIBRARY_PATH=$ZLIB_ROOT/lib:$LD_LIBRARY_PATH
export LD_LIBRARY_PATH=$PNG_ROOT/lib:$LD_LIBRARY_PATH
export LD_LIBRARY_PATH=$BLOSC_ROOT/lib:$LD_LIBRARY_PATH
export LD_LIBRARY_PATH=$PNGwriter_DIR/lib:$LD_LIBRARY_PATH

export PATH=$PNG_ROOT/bin:$PATH

export CMAKE_PREFIX_PATH=$ZLIB_ROOT:$CMAKE_PREFIX_PATH
export CMAKE_PREFIX_PATH=$PNG_ROOT:$CMAKE_PREFIX_PATH

export MPI_ROOT=$MPICH_DIR
export HDF5_ROOT=$HDF5_DIR

# Environment #################################################################
#
export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="cuda:60"

export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

# "tbg" default options #######################################################
#   - SLURM (sbatch)
#   - "normal" queue
export TBG_SUBMIT="sbatch"
export TBG_TPLFILE="etc/picongpu/pizdaint-cscs/normal.tpl"

# helper tools ################################################################

# allocate an interactive shell for one hour
#   getNode 2  # allocates two interactive nodes (default: 1)
getNode() {
    if [ -z "$1" ] ; then
        numNodes=1
    else
        numNodes=$1
    fi
    # --ntasks-per-core=2  # activates intel hyper threading
    salloc --time=1:00:00 --nodes="$numNodes" --ntasks-per-node=12 --ntasks-per-
↪core=2 --partition normal --gres=gpu:1 --constraint=gpu
}

# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

1.4.4 Taurus (TU Dresden)

System overview: link

User guide: link

Production directory: `/scratch/$USER/` and `/scratch/$proj/`

For these profiles to work, you need to download the *PIConGPU source code* and install *PNGwriter* manually.

Queue: gpu1 (Nvidia K20x GPUs)

```
# Name and Path of this Script ################################ (DO NOT change!)
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ################################# (edit the following lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on batch system jobs: NONE, BEGIN, END, FAIL, REQUEUE, ALL,
#     TIME_LIMIT, TIME_LIMIT_90, TIME_LIMIT_80 and/or TIME_LIMIT_50
export MY_MAILNOTIFY="NONE"
export MY_MAIL="someone@example.com"
export MY_NAME="$(whoami) <$MY_MAIL>"

# Project Information ######################################### (edit this line)
#   - project account for computing time
export proj=$(groups | awk '{print $1}')

# Text Editor for Tools ####################################### (edit this line)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
#export EDITOR="nano"

# Modules ######################################################################
#
module load modenv/scs5
module load foss/2018a
module load GCC/6.4.0-2.28
module load CMake/3.15.0-GCCcore-6.4.0
module load CUDA/9.2.88  # gcc <= 7, intel 15-17
module load OpenMPI/2.1.2-GCC-6.4.0-2.28

module load git/2.18.0-GCCcore-6.4.0
module load gnuplot/5.2.4-foss-2018a

module load Boost/1.66.0-foss-2018a
# currently not linking correctly:
#module load HDF5/1.10.1-foss-2018a
module load zlib/1.2.11-GCCcore-6.4.0

# module system does not export cmake prefix path:
export CMAKE_PREFIX_PATH=$EBROOTLIBPNG:$CMAKE_PREFIX_PATH
export CMAKE_PREFIX_PATH=$EBROOTZLIB:$CMAKE_PREFIX_PATH

# Environment ##################################################################
#

# path to own libraries:
export ownLibs=$HOME
# workaround HDF5:
export HDF5_ROOT=$ownLibs/lib/hdf5
export LD_LIBRARY_PATH=$HDF5_ROOT/lib:$LD_LIBRARY_PATH
export CMAKE_PREFIX_PATH=$HDF5_ROOT:$CMAKE_PREFIX_PATH
```

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```
# pngwriter needs to be built by the user:
export PNGwriter_DIR=$ownLibs/lib/pngwriter
export CMAKE_PREFIX_PATH=$PNGwriter_DIR:$CMAKE_PREFIX_PATH
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$PNGwriter_DIR/lib/

export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="cuda:35"

export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

# "tbg" default options ################################################
#   - SLURM (sbatch)
#   - "gpu1" queue
export TBG_SUBMIT="sbatch"
export TBG_TPLFILE="etc/picongpu/taurus-tud/k20x.tpl"

# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

Queue: gpu2 (Nvidia K80 GPUs)

```
# Name and Path of this Script ############################### (DO NOT change!)
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ################################# (edit the following lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on batch system jobs: NONE, BEGIN, END, FAIL, REQUEUE, ALL,
#     TIME_LIMIT, TIME_LIMIT_90, TIME_LIMIT_80 and/or TIME_LIMIT_50
export MY_MAILNOTIFY="NONE"
export MY_MAIL="someone@example.com"
export MY_NAME="$(whoami) <$MY_MAIL>"

# Project Information ######################################## (edit this line)
#   - project account for computing time
export proj=$(groups | awk '{print $1}')

# Text Editor for Tools ####################################### (edit this line)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
#export EDITOR="nano"

# Modules ######################################################################
#
module purge
module load modenv/scs5
module load gompic/2019b # loads GCC/8.3.0 CUDA/10.1.243 zlib/1.2.11 OpenMPI/3.1.4
# gompic/2020b does not have a corresponding boost module
module load CMake/3.15.3-GCCcore-8.3.0
module load Boost/1.71.0-gompic-2019b
module load git/2.23.0-GCCcore-8.3.0-nodocs
```

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```
module load libpng/1.6.37-GCCcore-8.3.0
module load HDF5/1.10.5-gompic-2019b
module load Python/3.7.4-GCCcore-8.3.0

# Self-Build Software #########################################################
#
# needs to be compiled by the user
# Check the install script at
# https://gist.github.com/steindev/86df43bef49586e2b33d2fb0a372f09c
#
# path to own libraries:
export PIC_LIBS=$HOME/lib

export BLOSC_ROOT=$PIC_LIBS/blosc-1.21.0
export LD_LIBRARY_PATH=$BLOSC_ROOT/lib:$LD_LIBRARY_PATH

export PNGwriter_ROOT=$PIC_LIBS/pngwriter-0.7.0
export CMAKE_PREFIX_PATH=$PNGwriter_ROOT:$CMAKE_PREFIX_PATH
export LD_LIBRARY_PATH=$PNGwriter_ROOT/lib:$LD_LIBRARY_PATH

export ADIOS2_ROOT=$PIC_LIBS/adios2-2.7.1
export LD_LIBRARY_PATH=$ADIOS2_ROOT/lib64:$LD_LIBRARY_PATH

export OPENPMD_ROOT=$PIC_LIBS/openpmd-0.14.1
export LD_LIBRARY_PATH=$OPENPMD_ROOT/lib64:$LD_LIBRARY_PATH


# Environment #################################################################
#
export PROJECT=/projects/$proj

export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="cuda:37"

export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

# "tbg" default options #######################################################
#   - SLURM (sbatch)
#   - "gpu2" queue
export TBG_SUBMIT="sbatch"
export TBG_TPLFILE="etc/picongpu/taurus-tud/k80.tpl"

alias getNode='srun -p gpu2-interactive --gres=gpu:4 -n 1 --pty --mem=0 -t 2:00:00␣
↪bash'

# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

Queue: knl (Intel Xeon Phi - Knights Landing)

For this profile, you additionally need to install your own *boost*.

```
# Name and Path of this Script ################################ (DO NOT change!)
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ################################ (edit the following lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on batch system jobs: NONE, BEGIN, END, FAIL, REQUEUE, ALL,
#     TIME_LIMIT, TIME_LIMIT_90, TIME_LIMIT_80 and/or TIME_LIMIT_50
export MY_MAILNOTIFY="NONE"
export MY_MAIL="someone@example.com"
export MY_NAME="$(whoami) <$MY_MAIL>"

# Project Information ######################################### (edit this line)
#   - project account for computing time
export proj=$(groups | awk '{print $1}')

# Text Editor for Tools ####################################### (edit this line)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
#export EDITOR="nano"

# Modules ######################################################################
#
module load modenv/scs5
module load iimpi/2018a
module load git/2.18.0-GCCcore-6.4.0
module load CMake/3.15.0-GCCcore-7.3.0
module load Boost/1.66.0-intel-2018a
module load HDF5/1.10.1-intel-2018a
module load libpng/1.6.34-GCCcore-7.3.0

# module system does not export cmake prefix path:
export CMAKE_PREFIX_PATH=$EBROOTLIBPNG:$CMAKE_PREFIX_PATH
export CMAKE_PREFIX_PATH=$EBROOTZLIB:$CMAKE_PREFIX_PATH

# Environment ##################################################################
#

# compilers are not set correctly by the module system:
export CC=`which icc`
export CXX=$CC

# path to own libraries:
export ownLibs=$HOME

export PNGwriter_DIR=$ownLibs/lib/pngwriter
export CMAKE_PREFIX_PATH=$PNGwriter_DIR:$CMAKE_PREFIX_PATH
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$PNGwriter_DIR/lib/

export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="omp2b:MIC-AVX512"

export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

# "tbg" default options ########################################################
```

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```
#   - SLURM (sbatch)
#   - "knl" queue
export TBG_SUBMIT="sbatch"
export TBG_TPLFILE="etc/picongpu/taurus-tud/knl.tpl"

alias getNode='srun -p knl -N 1 -c 64 --mem=90000 --constraint="Quadrant&Cache" --
↪pty bash'

# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

Queue: ml (NVIDIA V100 GPUs on Power9 nodes)

For this profile, you additionally need to compile and install everything for the power9-architecture including your own *boost*, *HDF5*, c-blosc and *ADIOS*.

Note: Please find a Taurus ml quick start here.

Note: You need to compile the libraries and PIConGPU on an `ml` node since only nodes in the `ml` queue are Power9 systems.

```
# Name and Path of this Script ################################ (DO NOT change!)
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ################################# (edit the following lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on batch system jobs: NONE, BEGIN, END, FAIL, REQUEUE, ALL,
#     TIME_LIMIT, TIME_LIMIT_90, TIME_LIMIT_80 and/or TIME_LIMIT_50
export MY_MAILNOTIFY="NONE"
export MY_MAIL="someone@example.com"
export MY_NAME="$(whoami) <$MY_MAIL>"

# Text Editor for Tools ########################################## (edit this line)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
#export EDITOR="nano"

# Modules ######################################################################
#
module switch modenv/ml

# load CUDA/9.2.88-GCC-7.3.0-2.30, also loads GCC/7.3.0-2.30, zlib, OpenMPI and␣
↪others
module load fosscuda/2018b
module load CMake/3.15.0-GCCcore-7.3.0
module load libpng/1.6.34-GCCcore-7.3.0

printf "@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@\n"
printf "@ Note: You need to compile picongpu on a node. @\n"
printf "@       Likewise for building the libraries.    @\n"
printf "@       Get a node with the getNode command.    @\n"
printf "@       Then source %s again.@\n" "$(basename $PIC_PROFILE)"
```

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```
printf "@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@\n"

# Self-Build Software ##########################################################
#
# needs to be compiled by the user
# Check the install script at
# https://gist.github.com/steindev/cc02eae81f465833afa27fc8880f3473#file-picongpu_
↪0-4-3_taurus-tud-sh
#
export PIC_LIBS=$HOME/lib/power9
export BOOST_ROOT=$PIC_LIBS/boost-1.68.0-Power9
export PNGwriter_DIR=$PIC_LIBS/pngwriter-0.7.0-Power9
export HDF5_ROOT=$PIC_LIBS/hdf5-1.8.20-Power9
export BLOSC_ROOT=$PIC_LIBS/blosc-1.16.2-Power9

export LD_LIBRARY_PATH=$BOOST_ROOT/lib:$LD_LIBRARY_PATH
export LD_LIBRARY_PATH=$PNGwriter_DIR/lib:$LD_LIBRARY_PATH
export LD_LIBRARY_PATH=$HDF5_ROOT/lib:$LD_LIBRARY_PATH
export LD_LIBRARY_PATH=$BLOSC_ROOT/lib:$LD_LIBRARY_PATH
export CMAKE_PREFIX_PATH=$HDF5_ROOT:$CMAKE_PREFIX_PATH

export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="cuda:70"

export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

# python not included yet
export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

# This is necessary in order to make alpaka compile.
# The workaround is from Axel Huebl according to alpaka PR #702.
export CXXFLAGS="-Dlinux"

# "tbg" default options ########################################################
#   - SLURM (sbatch)
#   - "ml" queue
export TBG_SUBMIT="sbatch"
export TBG_TPLFILE="etc/picongpu/taurus-tud/V100.tpl"

# allocate an interactive shell for two hours
#   getNode 2  # allocates 2 interactive nodes (default: 1)
function getNode() {
    if [ -z "$1" ] ; then
        numNodes=1
    else
        numNodes=$1
    fi
    export OMP_NUM_THREADS=7
    srun --time=2:00:00 --nodes=$numNodes --ntasks=$((6 * $numNodes)) --ntasks-per-
↪node=6 --cpus-per-task=7 --mem=0 --exclusive --gres=gpu:6 -p ml --pty bash
}

# allocate an interactive shell for two hours
#   getDevice 2  # allocates 2 interactive devices on one node (default: 1)
function getDevice() {
    if [ -z "$1" ] ; then
        numDevices=1
    else
```

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```
        if [ "$1" -gt 6 ] ; then
            echo "The maximal number of devices per node is 6." 1>&2
            return 1
        else
            numDevices=$1
        fi
    fi
    export OMP_NUM_THREADS=7
    srun --time=2:00:00 --nodes=1 --ntasks=$numDevices --ntasks-per-node=$((
↪$numDevices)) --cpus-per-task=7 --mem=$((254000 / $numDevices)) --gres=gpu:
↪$numDevices -p ml --pty bash
}

# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

1.4.5 Lawrencium (LBNL)

System overview: link

User guide: link

Production directory: `/global/scratch/$USER/`

For this profile to work, you need to download the *PIConGPU source code* and install *boost and PNGwriter* manually. Additionally, you need to make the `rsync` command available as written below.

```
# Name and Path of this Script ############################### (DO NOT change!)
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ################################# (edit the following lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on batch system jobs: NONE, BEGIN, END, FAIL, REQUEUE, ALL,
#     TIME_LIMIT, TIME_LIMIT_90, TIME_LIMIT_80 and/or TIME_LIMIT_50
export MY_MAILNOTIFY="NONE"
export MY_MAIL="someone@example.com"
export MY_NAME="$(whoami) <$MY_MAIL>"

# Text Editor for Tools ########################################## (edit this line)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
#export EDITOR="nano"

# Modules ######################################################################
#
if [ -f /etc/profile.d/modules.sh ]
then
        . /etc/profile.d/modules.sh
        module purge

        # Core Dependencies
        module load gcc
        module load cuda
        echo "WARNING: Boost version is too old! (Need: 1.65.1+)" >&2
        # module load boost/1.65.1-gcc
        module load openmpi/1.6.5-gcc
```

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```
        # Core tools
        module load git
        module load cmake
        module load python/2.6.6
        module load ipython/0.12 matplotlib/1.1.0 numpy/1.6.1 scipy/0.10.0

        # Plugins (optional)
        module load hdf5/1.8.11-gcc-p
        export CMAKE_PREFIX_PATH=$HOME/lib/pngwriter:$CMAKE_PREFIX_PATH
        export LD_LIBRARY_PATH=$HOME/lib/pngwriter/lib:$LD_LIBRARY_PATH

        # Debug Tools
        #module load valgrind/3.10.1
        #module load totalview/8.10.0-0

fi

# Environment ##################################################################
#
alias allocK20='salloc --time=0:30:00 --nodes=1 --ntasks-per-node=1 --cpus-per-
↪task=8 --partition lr_manycore'
alias allocFermi='salloc --time=0:30:00 --nodes=1 --ntasks-per-node=2 --cpus-per-
↪task=6 --partition mako_manycore'

export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="cuda:20"

# fix pic-create: re-enable rsync
#   ssh lrc-xfer.scs00
#   -> cp /usr/bin/rsync $HOME/bin/
export PATH=$HOME/bin:$PATH

export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

# "tbg" default options ########################################################
#   - SLURM (sbatch)
#   - fermi queue (also available: 2 K20 via k20.tpl)
export TBG_SUBMIT="sbatch"
export TBG_TPLFILE="etc/picongpu/lawrencium-lbnl/fermi.tpl"

# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

1.4.6 Cori (NERSC)

System overview: link

User guide: link

Production directory: `$SCRATCH` (link).

For these profiles to work, you need to download the *PIConGPU source code* and install *PNGwriter* manually.

Queue: regular (Intel Xeon Phi - Knights Landing)

```
# Name and Path of this Script ################################ (DO NOT change!)
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ################################# (edit the following lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on batch system jobs: NONE, BEGIN, END, FAIL, REQUEUE, ALL,
#     TIME_LIMIT, TIME_LIMIT_90, TIME_LIMIT_80 and/or TIME_LIMIT_50
export MY_MAILNOTIFY="NONE"
export MY_MAIL="someone@example.com"
export MY_NAME="$(whoami) <$MY_MAIL>"

# Project Information ######################################### (edit this line)
#   - project account for computing time
export proj="<yourProject>"

# Text Editor for Tools ####################################### (edit this line)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
#export EDITOR="nano"

# General modules ##############################################################
#
module swap craype-haswell craype-mic-knl
module swap PrgEnv-intel PrgEnv-gnu  # GCC 8.2.0
module load cmake/3.15.0
module load boost/1.70.0

# Other Software ###############################################################
#
module load cray-hdf5-parallel/1.10.2.0
module load png/1.6.34

export PNGwriter_ROOT=${HOME}/sw/pngwriter-0.7.0-21-g9dc58ed

# Environment ##################################################################
#
export CC="$(which cc)"
export CXX="$(which CC)"
export CRAYPE_LINK_TYPE=dynamic

export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="omp2b"  # usually ":MIC-AVX512" but we use PrgEnv wrappers

export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

# "tbg" default options ########################################################
#   - SLURM (sbatch)
#   - "defq" queue
export TBG_SUBMIT="sbatch"
export TBG_TPLFILE="etc/picongpu/cori-nersc/knl.tpl"

# allocate an interactive shell for one hour
#   getNode 2  # allocates two interactive nodes (default: 1)
```

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```
function getNode() {
    if [ -z "$1" ] ; then
        numNodes=1
    else
        numNodes=$1
    fi
    srun --time=1:00:00 --nodes=$numNodes --ntasks-per-node=1 --cpus-per-task=64 -
↪C "knl,quad,cache" -p regular --pty bash
}

# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

Queue: dgx (DGX - A100)

```
# Name and Path of this Script ################################ (DO NOT change!)
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ################################# (edit the following lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on batch system jobs: NONE, BEGIN, END, FAIL, REQUEUE, ALL,
#     TIME_LIMIT, TIME_LIMIT_90, TIME_LIMIT_80 and/or TIME_LIMIT_50
export MY_MAILNOTIFY="NONE"
export MY_MAIL="someone@example.com"
export MY_NAME="$(whoami) <$MY_MAIL>"

# Project Information ######################################### (edit this line)
#   - project account for computing time
export proj="<yourProject>"
# Project reservation (can be empty if no reservation exists)
export RESERVATION=""

# Text Editor for Tools ####################################### (edit this line)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
#export EDITOR="nano"

# General modules ##############################################################
#
module purge
module load dgx
module swap PrgEnv-intel PrgEnv-gnu
module load cuda openmpi
module load cmake/3.18.2
module load boost/1.70.0

# Other Software ###############################################################
#
module load png/1.6.34
module load zlib/1.2.11

export ADIOS2_ROOT=/global/cfs/cdirs/ntrain/dgx/openmpi/adios-2.7.1
export HDF5_ROOT=/global/cfs/cdirs/ntrain/dgx/openmpi/hdf5-1.10.7
export openPMD_ROOT=/global/cfs/cdirs/ntrain/dgx/openmpi/openPMD-api-0.13.4
export PNGwriter_ROOT=/global/cfs/cdirs/ntrain/dgx/pngwriter-0.7.0-25-g0c30be5
```

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```
# Environment ##################################################################
#
export CC="$(which gcc)"
export CXX="$(which g++)"
export CUDACXX=$(which nvcc)
export CUDAHOSTCXX=$(which g++)

export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="cuda:80"

export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

export LD_LIBRARY_PATH=$ADIOS2_ROOT/lib64:$HDF5_ROOT/lib:$openPMD_ROOT/lib64:
↪$PNGwriter_ROOT/lib64:$LD_LIBRARY_PATH
export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

# "tbg" default options ########################################################
#   - SLURM (sbatch)
#   - "defq" queue
export TBG_SUBMIT="sbatch"
export TBG_TPLFILE="etc/picongpu/cori-nersc/a100.tpl"

if [ -z "$RESERVATION" ] ; then
  SLURM_RESERVATION=""
else
  SLURM_RESERVATION="--reservation=$RESERVATION"
fi

# allocate an interactive node for one hour to execute a mpi parallel application
#   getNode 2  # allocates two interactive A100 GPUs (default: 1)
function getNode() {
    if [ -z "$1" ] ; then
        numNodes=1
    else
        numNodes=$1
    fi
    echo "Hint: please use 'srun --cpu_bind=cores <COMMAND>' for launching␣
↪multiple processes in the interactive mode."
    echo "             use 'srun -n 1 --pty bash' for launching a interactive␣
↪shell for compiling."
    salloc --time=1:00:00 --nodes=$numNodes --ntasks-per-node 8 --gpus 8 --cpus-
↪per-task=16 -A $proj -C dgx -q shared $SLURM_RESERVATION
}

# allocate an interactive device for one hour to execute a mpi parallel application
#   getDevice 2  # allocates two interactive devices (default: 1)
function getDevice() {
    if [ -z "$1" ] ; then
        numGPUs=1
    else
        if [ "$1" -gt 8 ] ; then
            echo "The maximal number of devices per node is 8." 1>&2
            return 1
        else
            numGPUs=$1
        fi
    fi
```

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```
    echo "Hint: please use 'srun --cpu_bind=cores <COMMAND>' for launching␣
↪multiple processes in the interactive mode."
    echo "             use 'srun -n 1 --pty bash' for launching a interactive␣
↪shell for compiling."
    salloc --time=1:00:00 --ntasks-per-node=$numGPUs --cpus-per-task=16 --gpus=
↪$numGPUs --mem=$((1010000 / 8) * $numGPUs) -A $proj -C dgx -q shared $SLURM_
↪RESERVATION
}

# allocate an interactive shell for compilation (without gpus)
function getShell() {
    srun --time=1:00:00 --nodes=1 --ntasks 1 --cpus-per-task=16 -A $proj -C dgx -q␣
↪shared $SLURM_RESERVATION --pty bash
}

# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

1.4.7 Draco (MPCDF)

System overview: link

User guide: link

Production directory: `/ptmp/$USER/`

For this profile to work, you need to download the *PIConGPU source code* and install *libpng and PNGwriter* manually.

```
# Name and Path of this Script ############################### (DO NOT change!)
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ################################# (edit the following lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on batch system jobs: NONE, BEGIN, END, FAIL, REQUEUE, ALL,
#     TIME_LIMIT, TIME_LIMIT_90, TIME_LIMIT_80 and/or TIME_LIMIT_50
export MY_MAILNOTIFY="NONE"
export MY_MAIL="someone@example.com"
export MY_NAME="$(whoami) <$MY_MAIL>"

# Text Editor for Tools ###################################### (edit this line)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
#export EDITOR="nano"

# General Modules ###############################################################
#
module purge

module load git/2.14
module load gcc/6.3
module load cmake/3.15.0
module load boost/gcc/1.64
module load impi/2017.3
module load hdf5-mpi/gcc/1.8.18
```

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```
# Other Software ##############################################################
#
# needs to be compiled by the user
export PNGWRITER_ROOT=$HOME/lib/pngwriter-0.7.0

export LD_LIBRARY_PATH=$PNGWRITER_ROOT/lib:$LD_LIBRARY_PATH
export LD_LIBRARY_PATH=$BOOST_HOME/lib:$LD_LIBRARY_PATH
export LD_LIBRARY_PATH=$HDF5_HOME/lib:$LD_LIBRARY_PATH
export LD_LIBRARY_PATH=$I_MPI_ROOT/lib64:$LD_LIBRARY_PATH

export HDF5_ROOT=$HDF5_HOME

export CXX=$(which g++)
export CC=$(which gcc)

# PIConGPU Helper Variables ###################################################
#
export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="omp2b:haswell"

export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

# "tbg" default options #######################################################
#   - SLURM (sbatch)
#   - "normal" queue
export TBG_SUBMIT="sbatch"
export TBG_TPLFILE="etc/picongpu/draco-mpcdf/general.tpl"

# helper tools ################################################################

# allocate an interactive shell for one hour
alias getNode='salloc --time=1:00:00 --nodes=1 --exclusive --ntasks-per-node=2 --
↪cpus-per-task=32 --partition general'

# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

1.4.8 D.A.V.I.D.E (CINECA)

System overview: link

User guide: link

Production directory: `$CINECA_SCRATCH/` (link)

For this profile to work, you need to download the *PIConGPU source code* manually.

Queue: dvd_usr_prod (Nvidia P100 GPUs)

```
# Name and Path of this Script ################################ (DO NOT change!)
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ################################ (edit the following lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on batch system jobs: NONE, BEGIN, END, FAIL, REQUEUE, ALL,
#     TIME_LIMIT, TIME_LIMIT_90, TIME_LIMIT_80 and/or TIME_LIMIT_50
export MY_MAILNOTIFY="NONE"
export MY_MAIL="someone@example.com"
export MY_NAME="$(whoami) <$MY_MAIL>"

# Project Information ######################################## (edit this line)
#   - project account for computing time
export proj=$(groups | awk '{print $2}')

# Text Editor for Tools ####################################### (edit this line)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
#export EDITOR="nano"

# General modules ##############################################################
#
module purge
module load gnu/6.4.0
module load cmake/3.15.0
module load cuda/9.2.88
module load openmpi/3.1.0--gnu--6.4.0
module load boost/1.68.0--openmpi--3.1.0--gnu--6.4.0

export CMAKE_PREFIX_PATH=$CUDA_HOME:$OPENMPI_HOME:$CMAKE_PREFIX_PATH
export CMAKE_PREFIX_PATH=$BOOST_HOME:$CMAKE_PREFIX_PATH

# Other Software ###############################################################
#
module load zlib/1.2.11--gnu--6.4.0
module load szip/2.1.1--gnu--6.4.0
module load blosc/1.12.1--gnu--6.4.0

module load hdf5/1.10.4--openmpi--3.1.0--gnu--6.4.0

module load libpng/1.6.35--gnu--6.4.0
module load freetype/2.9.1--gnu--6.4.0
module load pngwriter/0.7.0--gnu--6.4.0

export CMAKE_PREFIX_PATH=$ZLIB_HOME:$SZIP_HOME:$BLOSC_HOME:$CMAKE_PREFIX_PATH
export CMAKE_PREFIX_PATH=$LIBPNG_HOME:$FREETYPE_HOME:$PNGWRITER_HOME:$CMAKE_PREFIX_
↪PATH

# Work-Arounds #################################################################
#
# fix for Nvidia NVCC bug id 2448610
# see https://github.com/ComputationalRadiationPhysics/alpaka/issues/701
export CXXFLAGS="-Dlinux"

# Environment ##################################################################
#
#export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$BOOST_LIB

export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="cuda:60"
```

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```
export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

# "tbg" default options ################################################
#   - SLURM (sbatch)
#   - "gpu" queue
export TBG_SUBMIT="sbatch"
export TBG_TPLFILE="etc/picongpu/davide-cineca/gpu.tpl"

# allocate an interactive shell for one hour
#   getNode 2  # allocates two interactive nodes (default: 1)
function getNode() {
    if [ -z "$1" ] ; then
        numNodes=1
    else
        numNodes=$1
    fi
    srun --time=0:30:00 --nodes=$numNodes --ntasks-per-socket=8 --ntasks-per-
↪node=16 --mem=252000 --gres=gpu:4 -A $proj -p dvd_usr_prod --pty bash
}

# allocate an interactive shell for one hour
#   getDevice 2  # allocates two interactive devices (default: 1)
function getDevice() {
    if [ -z "$1" ] ; then
        numGPUs=1
    else
        if [ "$1" -gt 4 ] ; then
            echo "The maximal number of devices per node is 4." 1>&2
            return 1
        else
            numGPUs=$1
        fi
    fi
    srun  --time=1:00:00 --ntasks-per-node=$numGPUs --cpus-per-task=$((4 *
↪$numGPUs)) --gres=gpu:$numGPUs --mem=$((63000 * numGPUs)) -A $proj -p dvd_usr_
↪prod --pty bash
}

# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

1.4.9 JURECA (JSC)

System overview: link

User guide: link

Production directory: `$SCRATCH` (link)

For these profiles to work, you need to download the *PIConGPU source code* and install *PNGwriter and openPMD*, for the gpus partition also *Boost and HDF5*, manually.

Queue: batch (2 x Intel Xeon E5-2680 v3 CPUs, 12 Cores + 12 Hyperthreads/CPU)

```
# Name and Path of this Script ################################ (DO NOT change!)
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ################################ (edit the following lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on batch system jobs: NONE, BEGIN, END, FAIL, REQUEUE, ALL,
#     TIME_LIMIT, TIME_LIMIT_90, TIME_LIMIT_80 and/or TIME_LIMIT_50
export MY_MAILNOTIFY="NONE"
export MY_MAIL="someone@example.com"
export MY_NAME="$(whoami) <$MY_MAIL>"

# Project Information ######################################## (edit this line)
#   - project account for computing time
export proj=$(groups | awk '{print $5}')

# Text Editor for Tools ####################################### (edit this line)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
#export EDITOR="nano"

# Set up environment, including $SCRATCH and $PROJECT
jutil env activate -p $proj

# General modules ##############################################################
#
module purge
module load Intel/2019.0.117-GCC-7.3.0
module load CMake/3.15.0
module load IntelMPI/2018.4.274
module load Python/3.6.6
module load Boost/1.68.0-Python-3.6.6

# Other Software ###############################################################
#
module load zlib/.1.2.11
module load HDF5/1.10.1
module load libpng/.1.6.35
export CMAKE_PREFIX_PATH=$EBROOTZLIB:$EBROOTLIBPNG:$CMAKE_PREFIX_PATH

PARTITION_LIB=$PROJECT/lib_batch
PNGWRITER_ROOT=$PARTITION_LIB/pngwriter
export CMAKE_PREFIX_PATH=$PNGWRITER_ROOT:$CMAKE_PREFIX_PATH

BLOSC_ROOT=$PARTITION_LIB/c-blosc
export CMAKE_PREFIX_PATH=$BLOSC_ROOT:$CMAKE_PREFIX_PATH
export LD_LIBRARY_PATH=$BLOSC_ROOT/lib:$LD_LIBRARY_PATH

# Environment ##################################################################
#
#export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$BOOST_LIB

export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="omp2b:haswell"

export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

export CC=$(which icc)
export CXX=$(which icpc)
```

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```
export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

# "tbg" default options ###############################################################
#   - SLURM (sbatch)
#   - "batch" queue
export TBG_SUBMIT="sbatch"
export TBG_TPLFILE="etc/picongpu/jureca-jsc/batch.tpl"

# allocate an interactive shell for one hour
#   getNode 2  # allocates 2 interactive nodes (default: 1)
function getNode() {
    if [ -z "$1" ] ; then
        numNodes=1
    else
        numNodes=$1
    fi
    if [ $numNodes -gt 8 ] ; then
        echo "The maximal number of interactive nodes is 8." 1>&2
        return 1
    fi
    echo "Hint: please use 'srun --cpu_bind=sockets <COMMAND>' for launching␣
↪multiple processes in the interactive mode"
    export OMP_NUM_THREADS=24
    salloc --time=1:00:00 --nodes=$numNodes --ntasks-per-node=2 --mem=126000 -A
↪$proj -p devel bash
}

# allocate an interactive shell for one hour
#   getDevice 2  # allocates 2 interactive devices (default: 1)
function getDevice() {
    if [ -z "$1" ] ; then
        numDevices=1
    else
        if [ "$1" -gt 2 ] ; then
            echo "The maximal number of devices per node is 2." 1>&2
            return 1
        else
            numDevices=$1
        fi
    fi
    echo "Hint: please use 'srun --cpu_bind=sockets <COMMAND>' for launching␣
↪multiple processes in the interactive mode"
    export OMP_NUM_THREADS=24
    salloc --time=1:00:00 --ntasks-per-node=$(($numDevices)) --mem=126000 -A $proj␣
↪-p devel bash
}

# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

Queue: gpus (2 x Nvidia Tesla K80 GPUs)

```
# Name and Path of this Script ############################## (DO NOT change!)
```

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```
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ################################# (edit the following lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on batch system jobs: NONE, BEGIN, END, FAIL, REQUEUE, ALL,
#     TIME_LIMIT, TIME_LIMIT_90, TIME_LIMIT_80 and/or TIME_LIMIT_50
export MY_MAILNOTIFY="NONE"
export MY_MAIL="someone@example.com"
export MY_NAME="$(whoami) <$MY_MAIL>"

# Project Information ######################################## (edit this line)
#   - project account for computing time
export proj=$(groups | awk '{print $5}')

# Text Editor for Tools ####################################### (edit this line)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
#export EDITOR="nano"

# Set up environment, including $SCRATCH and $PROJECT
jutil env activate -p $proj

# General modules ##############################################################
#
module purge
module load GCC/7.3.0
module load CUDA/9.2.88
module load CMake/3.15.0
module load MVAPICH2/2.3-GDR
module load Python/3.6.6

# Other Software ###############################################################
#
module load zlib/.1.2.11
module load libpng/.1.6.35
export CMAKE_PREFIX_PATH=$EBROOTZLIB:$EBROOTLIBPNG:$CMAKE_PREFIX_PATH

PARTITION_LIB=$PROJECT/lib_gpus
BOOST_ROOT=$PARTITION_LIB/boost
export CMAKE_PREFIX_PATH=$BOOST_ROOT:$CMAKE_PREFIX_PATH
export LD_LIBRARY_PATH=$BOOST_ROOT/lib:$LD_LIBRARY_PATH

HDF5_ROOT=$PARTITION_LIB/hdf5
export PATH=$HDF5_ROOT/bin:$PATH
export CMAKE_PREFIX_PATH=$HDF5_ROOT:$CMAKE_PREFIX_PATH
export LD_LIBRARY_PATH=$HDF5_ROOT/lib:$LD_LIBRARY_PATH

PNGWRITER_ROOT=$PARTITION_LIB/pngwriter
export CMAKE_PREFIX_PATH=$PNGWRITER_ROOT:$CMAKE_PREFIX_PATH

BLOSC_ROOT=$PARTITION_LIB/c-blosc
export CMAKE_PREFIX_PATH=$BLOSC_ROOT:$CMAKE_PREFIX_PATH
export LD_LIBRARY_PATH=$BLOSC_ROOT/lib:$LD_LIBRARY_PATH

# Environment ##################################################################
#
#export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$BOOST_LIB

export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="cuda:37" # Nvidia K80 architecture
```

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```
export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

# "tbg" default options ################################################
#   - SLURM (sbatch)
#   - "gpus" queue
export TBG_SUBMIT="sbatch"
export TBG_TPLFILE="etc/picongpu/jureca-jsc/gpus.tpl"

# allocate an interactive shell for one hour
#   getNode 2  # allocates 2 interactive nodes (default: 1)
function getNode() {
    if [ -z "$1" ] ; then
        numNodes=1
    else
        numNodes=$1
    fi
    if [ $numNodes -gt 8 ] ; then
        echo "The maximal number of interactive nodes is 8." 1>&2
        return 1
    fi
    echo "Hint: please use 'srun --cpu_bind=sockets <COMMAND>' for launching␣
↪multiple processes in the interactive mode"
    salloc --time=1:00:00 --nodes=$numNodes --ntasks-per-node=4 --gres=gpu:4 --
↪mem=126000 -A $proj -p develgpus bash
}

# allocate an interactive shell for one hour
#   getDevice 2  # allocates 2 interactive devices (default: 1)
function getDevice() {
    if [ -z "$1" ] ; then
        numDevices=1
    else
        if [ "$1" -gt 4 ] ; then
            echo "The maximal number of devices per node is 4." 1>&2
            return 1
        else
            numDevices=$1
        fi
    fi
    echo "Hint: please use 'srun --cpu_bind=sockets <COMMAND>' for launching␣
↪multiple processes in the interactive mode"
    salloc --time=1:00:00 --ntasks-per-node=$(($numDevices)) --gres=gpu:4 --
↪mem=126000 -A $proj -p develgpus bash
}

# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

Queue: booster (Intel Xeon Phi 7250-F, 68 cores + Hyperthreads)

```
# Name and Path of this Script ################################ (DO NOT change!)
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ################################# (edit the following lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on batch system jobs: NONE, BEGIN, END, FAIL, REQUEUE, ALL,
#     TIME_LIMIT, TIME_LIMIT_90, TIME_LIMIT_80 and/or TIME_LIMIT_50
export MY_MAILNOTIFY="NONE"
export MY_MAIL="someone@example.com"
export MY_NAME="$(whoami) <$MY_MAIL>"

# Project Information ######################################## (edit this line)
#   - project account for computing time
export proj=$(groups | awk '{print $5}')

# Text Editor for Tools ####################################### (edit this line)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
#export EDITOR="nano"

# Set up environment, including $SCRATCH and $PROJECT
jutil env activate -p $proj

# General modules ##############################################################
#
module purge
module load Architecture/KNL
module load Intel/2019.0.117-GCC-7.3.0
module load CMake/3.15.0
module load IntelMPI/2018.4.274
module load Python/3.6.6
module load Boost/1.68.0-Python-3.6.6

# Other Software ###############################################################
#
module load zlib/.1.2.11
module load HDF5/1.10.1
module load libpng/.1.6.35
export CMAKE_PREFIX_PATH=$EBROOTZLIB:$EBROOTLIBPNG:$CMAKE_PREFIX_PATH

PARTITION_LIB=$PROJECT/lib_booster
PNGWRITER_ROOT=$PARTITION_LIB/pngwriter
export CMAKE_PREFIX_PATH=$PNGWRITER_ROOT:$CMAKE_PREFIX_PATH

BLOSC_ROOT=$PARTITION_LIB/c-blosc
export CMAKE_PREFIX_PATH=$BLOSC_ROOT:$CMAKE_PREFIX_PATH
export LD_LIBRARY_PATH=$BLOSC_ROOT/lib:$LD_LIBRARY_PATH

# Environment ##################################################################
#
#export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$BOOST_LIB

export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="omp2b:MIC-AVX512"

export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

export CC=$(which icc)
```

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```
export CXX=$(which icpc)

export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

# "tbg" default options ################################################
#   - SLURM (sbatch)
#   - "booster" queue
export TBG_SUBMIT="sbatch"
export TBG_TPLFILE="etc/picongpu/jureca-jsc/booster.tpl"

# allocate an interactive shell for one hour
#   getNode 2  # allocates 2 interactive nodes (default: 1)
function getNode() {
    if [ -z "$1" ] ; then
        numNodes=1
    else
        numNodes=$1
    fi
    if [ $numNodes -gt 8 ] ; then
        echo "The maximal number of interactive nodes is 8." 1>&2
        return 1
    fi
    export OMP_NUM_THREADS=34
    salloc --time=1:00:00 --nodes=$numNodes --ntasks-per-node=4 --mem=94000 -A
↪$proj -p develbooster bash
}

# allocate an interactive shell for one hour
#   getDevice 2  # allocates 2 interactive devices (default: 1)
function getDevice() {
    if [ -z "$1" ] ; then
        numDevices=1
    else
        if [ "$1" -gt 1 ] ; then
            echo "The maximal number of devices per node is 4." 1>&2
            return 1
        else
            numDevices=$1
        fi
    fi
    export OMP_NUM_THREADS=34
    salloc --time=1:00:00 --ntasks-per-node=$(($numDevices)) --mem=94000 -A $proj -
↪p develbooster bash
}

# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

1.4.10 JUWELS (JSC)

System overview: link

User guide: link

Production directory: `$SCRATCH` (link)

For these profiles to work, you need to download the *PIConGPU source code* and install *PNGwriter and openPMD*, for the gpus partition also *Boost and HDF5*, manually.

Queue: batch (2 x Intel Xeon Platinum 8168 CPUs, 24 Cores + 24 Hyperthreads/CPU)

```
# Name and Path of this Script ################################ (DO NOT change!)
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ################################ (edit the following lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on batch system jobs: NONE, BEGIN, END, FAIL, REQUEUE, ALL,
#     TIME_LIMIT, TIME_LIMIT_90, TIME_LIMIT_80 and/or TIME_LIMIT_50
export MY_MAILNOTIFY="NONE"
export MY_MAIL="someone@example.com"
export MY_NAME="$(whoami) <$MY_MAIL>"

# Project Information ######################################### (edit this line)
#   - project and account for allocation
#
#   `jutil user projects` will return a table of project associations.
#   Each row contains: project,unixgroup,PI-uid,project-type,budget-accounts
#   We need the first and last entry.
#   Here: select the last available project.
#   Alternative: Set proj, account manually
export proj=$( jutil user projects --noheader | awk '{print $1}' | tail -n 1 )
export account=$(jutil user projects -n | awk '{print $NF}' | tail -n 1)
# Text Editor for Tools ####################################### (edit this line)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
#export EDITOR="nano"
# Set up environment, including $SCRATCH and $PROJECT
# Handle a case where the budgeting account is not set.
if [ $accountt = "-" ]; then
    jutil env activate --project $proj;
else
    jutil env activate --project $proj --budget $account
fi


# General modules ##############################################################
#
module purge
module load Intel/2020.2.254-GCC-9.3.0
module load CMake/3.18.0
module load IntelMPI/2019.8.254
module load Python/3.8.5

module load Boost/1.73.0

# Other Software ###############################################################
#
module load HDF5/1.10.6
#export CMAKE_PREFIX_PATH=$EBROOTZLIB:$EBROOTLIBPNG:$CMAKE_PREFIX_PATH

PARTITION_LIB=$PROJECT/lib_batch
PNGWRITER_ROOT=$PARTITION_LIB/pngwriter
export CMAKE_PREFIX_PATH=$PNGWRITER_ROOT:$CMAKE_PREFIX_PATH

BLOSC_ROOT=$PARTITION_LIB/c-blosc
export CMAKE_PREFIX_PATH=$BLOSC_ROOT:$CMAKE_PREFIX_PATH
export LD_LIBRARY_PATH=$BLOSC_ROOT/lib:$LD_LIBRARY_PATH
```

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```
# Environment ##################################################################
#
#export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$BOOST_LIB

export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="omp2b:skylake"

export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

export CC=$(which icc)
export CXX=$(which icpc)

export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

# "tbg" default options ########################################################
#   - SLURM (sbatch)
#   - "batch" queue
export TBG_SUBMIT="sbatch"
export TBG_TPLFILE="etc/picongpu/juwels-jsc/batch.tpl"

# allocate an interactive shell for one hour
#   getNode 2  # allocates 2 interactive nodes (default: 1)
function getNode() {
    if [ -z "$1" ] ; then
        numNodes=1
    else
        numNodes=$1
    fi
    if [ $numNodes -gt 8 ] ; then
        echo "The maximal number of interactive nodes is 8." 1>&2
        return 1
    fi
    echo "Hint: please use 'srun --cpu_bind=sockets <COMMAND>' for launching␣
↪multiple processes in the interactive mode"
    export OMP_NUM_THREADS=48
    salloc --time=1:00:00 --nodes=$numNodes --ntasks-per-node=2 --mem=94000 -A
↪$account -p batch bash
}

# allocate an interactive shell for one hour
#   getDevice 2  # allocates 2 interactive devices (default: 1)
function getDevice() {
    if [ -z "$1" ] ; then
        numDevices=1
    else
        if [ "$1" -gt 2 ] ; then
            echo "The maximal number of devices per node is 2." 1>&2
            return 1
        else
            numDevices=$1
        fi
    fi
    echo "Hint: please use 'srun --cpu_bind=sockets <COMMAND>' for launching␣
↪multiple processes in the interactive mode"
    export OMP_NUM_THREADS=48
    salloc --time=1:00:00 --ntasks-per-node=$(($numDevices)) --mem=94000 -A
↪$account -p batch bash
}
```

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```
# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

Queue: gpus (4 x Nvidia V100 GPUs)

```
# Name and Path of this Script ################################ (DO NOT change!)
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ################################ (edit the following lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on batch system jobs: NONE, BEGIN, END, FAIL, REQUEUE, ALL,
#     TIME_LIMIT, TIME_LIMIT_90, TIME_LIMIT_80 and/or TIME_LIMIT_50
export MY_MAILNOTIFY="NONE"
export MY_MAIL="someone@example.com"
export MY_NAME="$(whoami) <$MY_MAIL>"

# Project Information ######################################### (edit this line)
#   - project and account for allocation
#   jutil user projects will return a table of project associations.
#   Each row contains: project,unixgroup,PI-uid,project-type,budget-accounts
#   We need the first and last entry.
#   Here: select the last available project.
export proj=$( jutil user projects --noheader | awk '{print $1}' | tail -n 1 )
export account=$(jutil user projects -n | awk '{print $NF}' | tail -n 1)

# Text Editor for Tools ####################################### (edit this line)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
#export EDITOR="nano"

# Set up environment, including $SCRATCH and $PROJECT
# Handle a case where the budgeting account is not set.
if [ "$account" = "-" ]; then
    jutil env activate --project $proj;
else
    jutil env activate --project $proj --budget $account
fi

# General modules ##############################################################
#
module purge
module load GCC/9.3.0
module load CUDA/11.0
module load CMake/3.18.0
module load ParaStationMPI/5.4.7-1
module load mpi-settings/CUDA
module load Python/3.8.5

module load Boost/1.74.0
module load HDF5/1.10.6
# necessary for evaluations (NumPy, SciPy, Matplotlib, SymPy, Pandas, IPython)
module load SciPy-Stack/2020-Python-3.8.5

# Other Software ###############################################################
```

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```
#
# Manually installed libraries are stored in PARTITION_LIB
PARTITION_LIB=$PROJECT/lib_gpus


PNGWRITER_ROOT=$PARTITION_LIB/pngwriter
export CMAKE_PREFIX_PATH=$PNGWRITER_ROOT:$CMAKE_PREFIX_PATH

BLOSC_ROOT=$PARTITION_LIB/c-blosc
export CMAKE_PREFIX_PATH=$BLOSC_ROOT:$CMAKE_PREFIX_PATH
export LD_LIBRARY_PATH=$BLOSC_ROOT/lib:$LD_LIBRARY_PATH


# Environment ##################################################################
#

export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="cuda:70" # Nvidia V100 architecture

export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

# "tbg" default options ########################################################
#   - SLURM (sbatch)
#   - "gpus" queue
export TBG_SUBMIT="sbatch"
export TBG_TPLFILE="etc/picongpu/juwels-jsc/gpus.tpl"

# allocate an interactive shell for one hour
#   getNode 2  # allocates 2 interactive nodes (default: 1)
function getNode() {
    if [ -z "$1" ] ; then
        numNodes=1
    else
        numNodes=$1
    fi
    if [ $numNodes -gt 8 ] ; then
        echo "The maximal number of interactive nodes is 8." 1>&2
        return 1
    fi
    echo "Hint: please use 'srun --cpu_bind=sockets <COMMAND>' for launching␣
↪multiple processes in the interactive mode"
    salloc --time=1:00:00 --nodes=$numNodes --ntasks-per-node=4 --gres=gpu:4 --
↪mem=180000 -A $account -p gpus bash
}

# allocate an interactive shell for one hour
#   getDevice 2  # allocates 2 interactive devices (default: 1)
function getDevice() {
    if [ -z "$1" ] ; then
        numDevices=1
    else
        if [ "$1" -gt 4 ] ; then
            echo "The maximal number of devices per node is 4." 1>&2
            return 1
        else
            numDevices=$1
```

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```
        fi
    fi
    echo "Hint: please use 'srun --cpu_bind=sockets <COMMAND>' for launching␣
↪multiple processes in the interactive mode"
    salloc --time=1:00:00 --ntasks-per-node=$(($numDevices)) --gres=gpu:4 --
↪mem=180000 -A $account -p gpus bash
}

# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

1.4.11 ARIS (GRNET)

System overview: link

User guide: link

Production directory: `$WORKDIR` (link)

For these profiles to work, you need to download the *PIConGPU source code*.

Queue: gpu (2 x NVIDIA Tesla k40m GPUs)

```
# Name and Path of this Script ################################## (DO NOT change!)
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ############################################# (edit those lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on batch system jobs: NONE, BEGIN, END, FAIL, REQUEUE, ALL,
#     TIME_LIMIT, TIME_LIMIT_90, TIME_LIMIT_80 and/or TIME_LIMIT_50
export MY_MAILNOTIFY="NONE"
export MY_MAIL="your email"
export MY_NAME="Name, name <$MY_MAIL>"

# Project Information ########################################## (edit this line)
#   - project account for computing time
export proj=$(groups | awk '{print $2}')

# Text Editor for Tools ######################################## (edit this line)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
#export EDITOR="nano"

# General modules ###############################################################
#
module purge
module load gnu/6.4.0
module load cmake
module load cuda/9.2.148
module load make
module load utils
module load python/2.7.13
module load git
module load picongpu
#module load boost/1.62.0
```

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```
#module load hdf5/1.8.17/gnu
# Other Software ###################################################################
#
# module load zlib/1.2.8
# module load pngwriter/0.7.0
# module load hdf5-parallel/1.8.20

# Work-Arounds #####################################################################
#
# fix for Nvidia NVCC bug id 2448610
# see https://github.com/ComputationalRadiationPhysics/alpaka/issues/701
#export CXXFLAGS="-Dlinux"

# Environment ######################################################################
#

export CMAKE_PREFIX_PATH=$PICONGPUROOT
export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="cuda:35"

export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

#export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

# "tbg" default options ############################################################
#   - SLURM (sbatch)
#   - "gpu" queue
export TBG_SUBMIT="sbatch"
export TBG_TPLFILE="etc/picongpu/aris-grnet/gpu.tpl"

# allocate an interactive shell for one hour
#   getNode 2  # allocates two interactive nodes (default: 1)
function getNode() {
    if [ -z "$1" ] ; then
        numNodes=1
    else
        numNodes=$1
    fi
    srun --time=0:30:00 --nodes=$numNodes --ntasks-per-socket=8 --ntasks-per-
↪node=16 --mem=252000 --gres=gpu:4 -A $proj -p dvd_usr_prod --pty bash
}

# allocate an interactive shell for one hour
#   getDevice 2  # allocates two interactive devices (default: 1)
function getDevice() {
    if [ -z "$1" ] ; then
        numGPUs=1
    else
        if [ "$1" -gt 4 ] ; then
            echo "The maximal number of devices per node is 4." 1>&2
            return 1
        else
            numGPUs=$1
        fi
    fi
    srun  --time=1:00:00 --ntasks-per-node=$numGPUs --cpus-per-task=$((4 *
↪$numGPUs)) --gres=gpu:$numGPUs --mem=$((63000 * numGPUs)) -A $proj -p dvd_usr_
↪prod --pty bash
```

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```
}

# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

1.4.12 Ascent (ORNL)

System overview and user guide: link

Production directory: usually `$PROJWORK/$proj/` (as on summit link).

For this profile to work, you need to download the *PIConGPU source code* and install *openPMD-api and PNGwriter* manually or use pre-installed libraries in the shared project directory.

V100 GPUs (recommended)

```
# Name and Path of this Script ################################ (DO NOT change!)
export PIC_PROFILE=$(cd $(dirname $BASH_SOURCE) && pwd)"/"$(basename $BASH_SOURCE)

# User Information ################################ (edit the following lines)
#   - automatically add your name and contact to output file meta data
#   - send me a mail on job (-B)egin, Fi(-N)ish
export MY_MAILNOTIFY=""
export MY_MAIL="someone@example.com"
export MY_NAME="$(whoami) <$MY_MAIL>"

# Project Information ######################################### (edit this line)
#   - project account for computing time
# export proj=[TODO: fill with: `groups | awk '{print $2}'`]

# Text Editor for Tools ####################################### (edit this line)
#   - examples: "nano", "vim", "emacs -nw", "vi" or without terminal: "gedit"
#module load nano
#export EDITOR="emacs -nw"

# basic environment ############################################################
module load gcc/8.1.1
module load spectrum-mpi/10.3.1.2-20200121

export CC=$(which gcc)
export CXX=$(which g++)

# required tools and libs
module load git/2.20.1
module load cmake/3.18.2
module load cuda/11.2.0
module load boost/1.66.0

# plugins (optional) ###########################################################
module load hdf5/1.10.4
module load c-blosc/1.12.1 zfp/0.5.2 sz/2.0.2.0 lz4/1.8.1.2
module load adios2/2.7.0
module load zlib/1.2.11
module load libpng/1.6.34 freetype/2.9.1
```

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```
module load nsight-compute/2021.1.0

# shared libs
#export PIC_LIBS=$PROJWORK/$proj/picongpu/lib/

# openPMD-api
#export OPENPMD_ROOT=$PIC_LIBS/openPMD-api/
#export LD_LIBRARY_PATH=$OPENPMD_ROOT/lib64:$LD_LIBRARY_PATH

# pngWriter
#export CMAKE_PREFIX_PATH=$PIC_LIBS/pngwriter:$CMAKE_PREFIX_PATH
#export LD_LIBRARY_PATH=$PIC_LIBS/pngwriter/lib:$LD_LIBRARY_PATH


# helper variables and tools #################################################
export PICSRC=$HOME/src/picongpu
export PIC_EXAMPLES=$PICSRC/share/picongpu/examples
export PIC_BACKEND="cuda:70"

export PATH=$PATH:$PICSRC
export PATH=$PATH:$PICSRC/bin
export PATH=$PATH:$PICSRC/src/tools/bin

export PYTHONPATH=$PICSRC/lib/python:$PYTHONPATH

alias getNode="bsub -P $proj -W 2:00 -nnodes 1 -Is /bin/bash"

# "tbg" default options ######################################################
export TBG_SUBMIT="bsub"
export TBG_TPLFILE="etc/picongpu/ascent-ornl/gpu_batch.tpl"

# Load autocompletion for PIConGPU commands
BASH_COMP_FILE=$PICSRC/bin/picongpu-completion.bash
if [ -f $BASH_COMP_FILE ] ; then
    source $BASH_COMP_FILE
else
    echo "bash completion file '$BASH_COMP_FILE' not found." >&2
fi
```

1.5 Changelog

1.5.1 0.6.0

Date: 2021-12-21

C++14, New Solvers, I/O via openPMD API, HIP Support

This release switches to C++14 as minimum required version. Transition to C++17 is planned for upcoming releases.

We extended PIConGPU with a few new solvers. Binary collisions are now available. We added arbitrary-order FDTD Maxwell's solver. All field solvers are now compatible with perfectly matched layer absorber, which became default. Yee solver now supports incident field generation using total field/scattered field technique. We added Higuera-Cary particle pusher and improved compatibility of pushers with probe species. Implementation of particle boundaries was extended to support custom positions, reflecting and thermal boundary kinds were added.

With this release, PIConGPU fully switches to openPMD API library for performing I/O. The native HDF5 and ADIOS output plugins were replaced with a new openPMD plugin. All other plugins were updated to use openPMD API. Plugins generally support HDF5 and ADIOS2 backends of openPMD API, a user can choose file format based on their installation of openPMD API. We also added new plugins for SAXS and particle merging.

We added support for HIP as a computational backend. In particular, it allows running on AMD GPUs. Several performance optimizations were added. Some functors and plugins now have performance-influencing parameters exposed to a user.

The code was largely modernized and refactored, documentation was extended.

Thanks to Sergei Bastrakov, Kseniia Bastrakova, Brian Edward Marre, Alexander Debus, Marco Garten, Bernhard Manfred Gruber, Axel Huebl, Jakob Trojok, Jeffrey Kelling, Anton Lebedev, Felix Meyer, Paweł Ordyna, Franz Poeschel, Lennert Sprenger, Klaus Steiniger, Manhui Wang, Sebastian Starke, Maxence Thévenet, Richard Pausch, René Widera for contributions to this release!

Changes to "0.5.0"

User Input Changes:

- Remove HDF5 I/O plugin (replaced with new openPMD plugin) #3361
- Remove ADIOS I/O plugin (replaced with new openPMD plugin) #3691
- Decouple field absorber selection from field solver #3635
- Move all field absorber compile-time parameters to fieldAbsorber.param #3645
- Change default field absorber to PML #3672
- Change current interpolation from compile-time to command-line parameter #3552
- Remove directional splitting field solver #3363
- Remove compile-time movePoint value from grid.param #3793
- Switch to cupla math functions #3245
- Scale particle exchange buffer #3465
- Update to new mallocMC version and parameters #3856

New Features:

- PIC:
  - Add strategy parameter for current deposition algorithms #3221
  - Add Higuera-Cary particle pusher #3280 #3371
  - Add support for PML absorber with Lehe field solver #3301
  - Add support for Lehe field solver in 2D #3321
  - Add arbitrary-order FDTD field solver #3338
  - Add ionization current #3355
  - Add PML support to arbitrary-order FDTD field solver #3417
  - Faster TWTS laser implementation #3439
  - Parametrize FieldBackground for accuracy vs. memory #3527
  - Add a check for Debye length resolution #3446
  - Add user-defined iteration start pipeline
  - Add binary collisions #3416
  - Expose compute current worker multiplier #3539
  - Add a new way to generate incident field using TF/SF #3592
  - Add support for device oversubscription #3632
  - Signal handling #3633

  - Replace FromHDF5Impl density with FromOpenPMDImpl #3655
  - Introduce filtered particleToGrid algorithm #3574
  - Record probe data with all pushers #3714
  - Compatibility check for laser and field solver #3734
  - Extend particles::Manipulate with area parameter #3747
  - Enable runtime kernel mapping #3750
  - Optimize particle pusher kernel #3775
  - Enable particle boundaries at custom positions #3763 #3776
  - Adjust physics log output #3825
  - Add a new particle manipulator combining total cell offset and RNG #3832
  - Add reflective particle boundary conditions #3806
  - Add thermal particle boundary conditions #3858
  - HIP support #3356 #3456 #3500
- PMacc:
  - MPI direct support #3195
  - Improve output of kernel errors in PMacc with PMACC_BLOCKING_KERNEL=ON #3396
  - Optimize atomic functor for HIP #3457
  - Add device-side assert macro #3488
  - Add support for alpaka OpenMP target/OpenACC #3512
  - Additional debug info in guard check for supercell size #3267
  - Clarify error message and add comments in GameOfLife #3553
  - Print milliseconds in output #3606
  - Enable KernelShiftParticles to operate in guard area #3772
- plugins:
  - Add a new openPMD plugin to replace the native HDF5 and ADIOS1 ones #2966
  - Add probabilistic particle merger plugin #3227
  - Add SAXS plugin using electron density #3134
  - Add work distribution parameter in radiation plugin #3354
  - Add field solver parameters attribute to output #3364
  - Update required openPMD version to 0.12.0 #3405
  - Use Streaming API in openPMD plugin #3485
  - Make radiation Amplitude class template #3519
  - Add compatibility to ISAAC GLM #3498
  - Extend JSON patterns in openPMD plugin #3513
  - Compatibility to new unified ISAAC naming scheme #3545
  - Use span-based storeChunk API in openPMD plugin #3609
  - Optimize radiation plugin math #3711
  - Deactivate support for writing to ADIOS1 via the openPMD plugin #3395
  - Avoid hardcoding of floating-point type in openPMD plugin #3759

  - Add checkpointing of internal RNG states #3758
  - Make the span-based storeChunk API opt-in in various openPMD-based IO routines #3933
- tools:
  - Update to C++14 #3242
  - Add JetBrains project dir to .gitignore. #3265
  - Convert path to absolute inside tbg #3190
  - Add verbose output for openPMD-api #3281
  - Switch to openPMD API in `plot_chargeConservation_overTime.py` #3505
  - Switch to openPMD API in `plot_chargeConservation.py` #3504
  - Save the used cmakeFlags setup in output directory #3537
  - Add JUWELS Booster profile #3341
  - Check for doxygen style in CI #3629
  - Update Summit profile #3680
  - Remove old CI helper #3745
  - Remove uncrustify #3746
  - Add python env to gitignore #3805

Bug Fixes:

- PIC:
  - Fix compilation with clang-cuda and Boost #3295
  - Modify FreeFormulaImpl density profile to evalute a functor in centers of cells #3415
  - Fix deprecation warnings #3467
  - Fix the scheme of updating convolutional B in PML by half time step #3475
  - Fix and modernize the generation scheme for MPI communication tags #3558
  - Fix TWTS implementations #3704
  - Fix domain adjuster for absorber in case there is a single domain along a direction #3760
  - Fix unreachable code warnings #3575
  - Fix incorrect assignment of Jz in 2d EmZ implementation #3893
  - Fix restarting with moving window #3902
  - Fix performance issue with HIP 4.3+ #3903
  - Fix using host function in device code #3911
- PMacc:
  - Fix missing override for virtual functions #3315
  - Fix unsafe access to a vector in cuSTL MPI reduce #3332
  - Fix cuSTL CartBuffer dereferencing a null pointer when CUDA is enabled #3330
  - Remove usage of `atomicAddNoRet` for HIP 4.1 #3572
  - Fix compilation with icc #3628
  - Fix warning concerning used C++17 extension #3318
  - Fix unused variable warning #3803
- plugins:

  - Fix checkpointing and output of PML fields for uneven domains #3276
  - Fix warnings in the openPMD plugin #3289
  - fix clang-cuda compile #3314
  - Fix shared memory size in the PhaseSpace plugin #3333
  - Fix observation direction precision to use float_X #3638
  - Fix crash in output after moving window stopped #3743
  - Fix openPMD warning in XrayScatteringWriter #3358
  - Fix warning due to missing virtual destructor #3499
  - Fix warning due to missing override #3855
  - Remove deprecated openPMD::AccessType and replace with openPMD::Access #3373
  - Fix processing of outgoing particles by multi plugins #3619
  - Fix getting unitSI for amplitude #3688
  - Fix outdated exception message for openPMD plugin with ADIOS1 #3730
  - Remove ususued variable in ISAAC plugin #3756
  - Fix warning in radiation plugin #3771
  - Fix internal linkage of private JSON header in openPMD plugin #3863
  - Fix treatment of bool particle attributes in openPMD plugin #3890
  - Add missing communication in XrayScattering #3937
- tools:
  - Fix plotting tool for numerical heating #3324
  - Fix typos in pic-create output #3435
  - No more "-r" in spack load #3873
  - Fix docker recipe #3921
- Fix KHI for non-CUDA devices #3285
- Fix clang10-cuda compile #3310
- Fix segfault in thermal test #3517
- Fix jump on uninitialized variable #3523
- Fix EOF whitespace test #3555
- Disable PMacc runtime tests for HIP in CI #3650

Misc:

- refactoring:
  - PIC:
    * Use cupla instead of cuda prefix for function calls #3211
    * Abstract PML definitions from YeePML field solver #3283
    * Refactor implementations of derivatives and curls for fields #3309
    * Refactor Lehe solver to use the new derivative and curl functors #3317
    * Add pmacc functions to get basis unit vectors #3319
    * Refactor margin traits for field derivatives #3320
    * Add a new trait GetCellType of field solvers #3322

    * Remove outdated pmacc/nvidia/rng/* #3351
    * Add generic utilities to get absorber thickness #3348
    * Remove pmacc::memory::makeUnique #3353
    * Remove unused HasIonizersWithRNG and UsesRNG #3367
    * Cleanup particle shape structs #3376
    * Refactoring and cleanup of species.param #3431
    * Rename picongpu::MySimulation to picongpu::Simulation #3476
    * Avoid access to temporary variable #3508
    * Remove unused enum picongpu::FieldType #3556
    * Switch internal handling of current interpolation from compile-time to run-time #3551
    * Refactor and update comments of GetMargin #3564
    * Remove enum picongpu::CommunicationTag #3561
    * Add a version of GetTrait taking only field solver type as a parameter #3571
    * Remove interface `DataConnector::releaseData()` #3582
    * Remove unused directory pmacc/nvidia #3604
    * Rename picongpu::particles::CallFunctor to pmacc::functor::Call #3608
    * Refactor common field absorber implementation #3611
    * Move PML implementation to a separate directory #3617
    * Move the basic implementation of FDTD field solver to the new eponymous template #3643
    * Use IUnary with filters in collisions and FieldTmp #3687
    * Refactor field update functor #3648
    * Replace leftover usage of boost/type_traits with std:: counterparts #3812
    * Relocate function to move particles #3802
    * Fix a typo in domain adjuster output #3851
    * Replace C-style stdlib includes with C++ counterparts #3852
    * Replace raw pointers used for memory management with smart pointers #3854
    * Refactor and document laser profiles #3798
    * Remove unused variable boundaryKind #3769
  - PMacc:
    * Fix pedantic warnings #3255
    * Refactor ConstVector #3274
    * Set default values for some PMacc game of life example arguments #3352
    * Refactor PMacc warp and atomic functions #3343
    * Change SharedMemAllocator function qualifiers from DEVICEONLY to DINLINE #3520
    * Delete unused file MultiGridBuffer.hpp #3565
    * Refactor lockstep::ForEach #3630
    * Refactor lockstep programming #3616
    * Change ExchangeTypeToRank from protected to public #3718
    * Clarify naming and comments for pmacc kernel mapping types #3765

        * Separate notification of plugins into a new function in SimulationHelper #3788
        * Add a factory and a factory function for pmacc::StrideMapping #3785
        * Replace custom compile-time string creation by BOOST_METAPARSE_STRING #3792
        * Refactor CachedBox #3813
        * Refactor and extend Vector #3817
        * Drop unused TwistedAxesNavigator #3821
        * Refactor DataBox #3820
        * Replace PitchedBox ctor with offset by DataBox.shift() #3828
        * Rename type to Reference in Cursor #3827
        * Fix a warning in MapperConcept #3777
        * Remove leftover mentions of ADIOS1 #3795
    - plugins:
        * Remove unused ParticlePatches class #3419
        * Switch to openPMD API in PhaseSpace plugin #3468
        * Switch to openPMD API in MacroParticleCounter plugin #3570
        * Switch to openPMD API in ParticleCalorimeter plugin #3560
        * Vector field vis vis compatility and benchmarking in ISAAC plugin #3719
        * Remove libSplash #3744
        * Remove unnecessary parameter in writeField function template of openPMD plugin #3767
        * Remove –openPMD.compression parameter #3764
        * Rename instance interface for multiplugins #3822
        * Use multidim access instead of two subscripts #3829
        * Use Iteration::close() in openPMD plugin #3408
    - tools:
        * Add cmake option to enforce dependencies #3586
        * Update to mallocMC 2.5.0crp-dev #3325
        * Clarify output concerning cuda_memtest not being available #3345
    - Reduce complexity of examples #3323
    - Avoid species dependency in field solver compile test #3430
    - Switch from Boost tests to Catch2 #3447
    - Introduce clang format #3440
    - Use ubuntu 20.04 with CUDA 11.2 in docker image #3502
    - Apply sorting of includes according to clang-format #3605
    - Remove leftover boost::shared_ptr #3800
    - Modernize according to clang-tidy #3801
    - Remove more old boost includes and replace with std:: counterparts #3819
    - Remove boost::result_of #3830
    - Remove macro __deleteArray() #3839
- documentation:

- Fix a typo in the reference to [Pausch2018] #3214
- Remove old HZDR systems #3246
- Document C++14 requirement #3268
- Add reference in LCT Example #3297
- Fix minor issues with the sphinx rst formating #3290
- Fix the name of probe fieldE and fieldB attribute in docs #3385
- Improve clarity of comments concerning density calculation and profile interface #3414
- Clarify comments for generating momentums based on temperature #3423
- Replace travis badges with gitlab ones #3451
- Update supported CUDA versions #3458
- Juwels profile update #3359
- Extend reminder to load environment in the docs with instructions for spack #3478
- Fix typo in FieldAbsorberTest #3528
- Improve documentation of clang-format usage #3522
- Fix some outdated docs regarding output and checkpoint backends #3535
- Update version to 0.6.0-dev #3542
- Add installation instructions for ADIOS2 and HDF5 backends of openPMD API #3549
- Add support for boost 1.74.0 #3583
- Add brief user documentation for boundary conditions #3600
- Update grid.param file doxygen string #3601
- Add missing arbitrary order solver to the list of PML-enabled field solvers #3550
- Update documentation of AOFDTD #3578
- Update spack installation guide #3640
- Add fieldAbsorber runtime parameter to TBG_macros.cfg #3646
- Extend docs for the openPMD plugin regarding –openPMD.source #3667
- Update documentation of memory calculator #3669
- Summit template and documentation for asynchronous writing via ADIOS2 SST #3698
- Add DGX (A100) profile on Cori #3694
- Include clang-format in suggested contribution pipeline #3710
- Extend TBG_macros and help string for changing field absorber #3736
- Add link to conda picongpu-analysis-environment file to docs #3738
- Add a brief doc page on ways of adding a laser to a simulation #3739
- Update cupla to 0.3.0 release #3748
- Update to malloc mc2.6.0crp-dev #3749
- Mark openPMD backend libraries as optional dependencies in the docs #3752
- Add a documentation page for developers that explains how to extend PIConGPU #3791
- Extend doc section on particle filter workflows #3782
- Add clarification on pluginUnload #3836
- Add a readthedocs page on debugging #3848

  - Add a link to the domain definitions wiki in the particle global filter workflow #3849
  - add reference list #3273
  - Fix docker documentation #3544
  - Extend comments of CreateDensity #3837
  - Refactor and document laser profiles #3798
  - Mark CUDA 11.2 as supported version #3503
  - Document intention of Pointer #3831
  - Update ISAAC plugin documentation #3740
  - Add a doxygen warning to not remove gamma filter in transition radiation #3857
  - Extend user documentation with a warning about tools being Linux-only #3462
- Update hemera modules and add openPMDapi module #3270
- Separate project and account for Juwels profile #3369
- Adjust tpl for juwels #3368
- Delete superfluous `fieldSolver.param` in examples #3374
- Build CI tests with all dependencies #3316
- Update openPMD and ADIOS module #3393
- Update summit profile to include openPMD #3384
- Add both adios and adios2 module on hemera #3411
- Use openPMD::getVersion() function #3427
- Add SPEC benchmark example #3466
- Update the FieldAbsorberTest example to match the Taflove book #3487
- Merge mainline changes back into dev #3540
- SPEC bechmark: add new configurations #3597
- Profile for spock at ORNL #3627
- CI: use container version 1.3 #3644
- Update spock profile #3653
- CI: use HIP 4.2 #3662
- Compile for MI100 architecture only using spock in ORNL #3671
- Fix compile warning using spock in ORNL #3670
- Add radiation cases to SPEC benchmark #3683
- Fix taurus-tud k80 profile #3729
- Update spock profile after update to RHEL8 #3755
- Allow interrupting job in CI #3761
- Fix drift manipulator in SingleParticle example #3766
- Compile on x86 runners in CI #3762
- Update gitignore for macOS system generated files #3779
- Use stages for downstream pipe in CI #3773
- Add Acceleration pusher to compile-time test suite #3844
- Update mallocMC #3897

1.5.2 0.5.0

Date: 2020-06-03

Perfectly Matched Layer (PML) and Bug Fixes

This release adds a new field absorber for the Yee solver, convolutional perfectly matched layer (PML). Compared to the still supported exponential dampling absorber, PML provides better absorption rate and much less spurious reflections.

We added new plugins for computing emittance and transition radiation, particle rendering with the ISAAC plugin, Python tools for reading and visualizing output of a few plugins.

The release also adds a few quality-of-life features, including a new memory calculator, better command-line experience with new options and bashcompletion, improved error handling, cleanup of the example setups, and extensions to documentation.

Thanks to Igor Andriyash, Sergei Bastrakov, Xeinia Bastrakova, Andrei Berceanu, Finn-Ole Carstens, Alexander Debus, Jian Fuh Ong, Marco Garten, Axel Huebl, Sophie Rudat (Koßagk), Anton Lebedev, Felix Meyer, Pawel Ordyna, Richard Pausch, Franz Pöschel, Adam Simpson, Sebastian Starke, Klaus Steiniger, René Widera for contributions to this release!

Changes to "0.4.0"

User Input Changes:

- Particle pusher acceleration #2731
- stop moving window after N steps #2792
- Remove unused ABSORBER_FADE_IN_STEPS from .param files in examples #2942
- add namespace "radiation" around code related to radiation plugin #3004
- Add a runtime parameter for window move point #3022
- Ionization: add silicon to pre-defines #3078
- Make dependency between boundElectrons and atomicNumbers more explicit #3076
- openPMD: use particle id naming #3165
- Docs: update `species.param` #2793 #2795

New Features:

- PIC:
  - Particle pusher acceleration #2731
  - Stop moving window after N steps #2792
  - Auto domain adjustment #2840
  - Add a wrapper around main() to catch and report exceptions #2962
  - Absorber perfectly matched layer PML #2950 #2967
  - Make dependency between boundElectrons and atomicNumbers more explicit #3076
- PMacc:
  - `ExchangeTypeNames` Verify Parameter for Access #2926
  - Name directions in species buffer warnings #2925
  - Add an implementation of exp for pmacc vectors #2956
  - SimulationFieldHelper: getter method to access cell description #2986
- plugins:

  - PhaseSpaceData: allow multiple iterations #2754
  - Python MPL Visualizer: plot for several simulations #2762
  - Emittance Plugin #2588
  - DataReader: Emittance & PlotMPL: Emittance, SliceEmittance, EnergyWaterfall #2737
  - Isaac: updated for particle rendering #2940
  - Resource Monitor Plugin: Warnings #3013
  - Transition radiation plugin #3003
  - Add output and python module doc for radiation plugin #3052
  - Add reference to thesis for emittance plugin doc #3101
  - Plugins: ADIOS & PhaseSpace Wterminate #2817
  - Calorimeter Plugin: Document File Suffix #2800
  - Fix returning a stringstream by value #3251
- tools:
  - Support alpaka accelerator `threads` #2701
  - Add getter for omega and n to python module #2776
  - Python Tools: Incorporate sim_time into readers and visualizers #2779
  - Add PIConGPU memory calculator #2806
  - Python visualizers as jupyter widgets #2691
  - pic-configure: add `--force/-f` option #2901
  - Correct target thickness in memory calculator #2873
  - CMake: Warning in 3.14+ Cache List #3008
  - Add an option to account for PML in the memory calculator #3029
  - Update profile hemera-hzdr: CMake version #3059
  - Travis CI: OSX sed Support #3073
  - CMake: mark cuda 10.2 as tested #3118
  - Avoid bash completion file path repetition #3136
  - Bashcompletion #3069
  - Jupyter widgets output capture #3149
  - Docs: Add ionization prediction plot #2870
  - pic-edit: clean cmake file cache if new param added #2904
  - CMake: Honor _ROOT Env Hints #2891
  - Slurm: Link stdout live #2839

Bug Fixes:

- PIC:
  - fix EveryNthCellImpl #2768
  - Split `ParserGridDistribution` into `hpp/cpp` file #2899
  - Add missing inline qualifiers potentially causing multiple definitions #3006
  - fix wrong used method prefix #3114
  - fix wrong constructor call #3117

  - Fix calculation of omega_p for logging #3163
  - Fix laser bug in case focus position is at the init plane #2922
  - Fix binomial current interpolation #2838
  - Fix particle creation if density zero #2831
  - Avoid two slides #2774
  - Fix warning: comparison of unsigned integer #2987
- PMacc:
  - Typo fix in Send/receive buffer warning #2924
  - Explicitly specify template argument for std::forward #2902
  - Fix signed int overflow in particle migration between supercells #2989
  - Boost 1.67.0+ Template Aliases #2908
  - Fix multiple definitions of PMacc identifiers and aliases #3036
  - Fix a compilation issue with ForEach lookup #2985
- plugins:
  - Fix misspelled words in plugin documentation #2705
  - Fix particle merging #2753
  - OpenMPI: Use ROMIO for IO #2857
  - Radiation Plugin: fix bool conditions for hdf5 output #3021
  - CMake Modules: Update ADIOS FindModule #3116
  - ADIOS Particle Writer: Fix timeOffset #3120
  - openPMD: use particle id naming #3165
  - Include int16 and uint16 types as traits for ADIOS #2929
  - Fix observation direction of transition radiation plugin #3091
  - Fix doc transition radiation plugin #3089
  - Fix doc rad plugin units and factors #3113
  - Fix wrong underline in TransRad plugin doc #3102
  - Fix docs for radiation in 2D #2772
  - Fix radiation plugin misleading filename #3019
- tools:
  - Update cuda_memtest: NVML Noise #2785
  - Dockerfile: No SSH Deamon & Keys, Fix Flex Build #2970
  - Fix hemera k80_restart.tpl #2938
  - Templates/profile for hemera k20 queue #2935
  - Splash2txt Build: Update deps #2914
  - splash2txt: fix file name trimming #2913
  - Fix compile splash2txt #2912
  - Docker CUDA Image: Hwloc Default #2906
  - Fix Python EnergyHistogramData: skip of first iteration #2799
- Spack: Fix Compiler Docs #2997

- Singularity: Workaround Chmod Issue, No UCX #3017
- Fix examples particle filters #3065
- Fix CUDA device selection #3084
- Fix 8.cfg for Bremsstrahlung example #3097
- Fix taurus profile #3152
- Fix a typo in density ratio value of the KHI example #3162
- Fix GCC constexpr lambda bug #3188
- CFL Static Assert: new grid.param #2804
- Fix missing exponent in fieldIonization.rst #2790
- Spack: Improve Bootstrap #2773
- Fix python requirements: remove sys and getopt #3172

Misc:

- refactoring:
  - PIC:
    - Eliminate M_PI (again) #2833
    - Fix MappingDesc name hiding #2835
    - More fixes for MSVC capturing constexpr in lambdas #2834
    - Core Particles: C++11 Using for Typedef #2859
    - Remove unused getCommTag() in FieldE, FieldB, FieldJ #2947
    - Add a using declaration for Difference type to yee::Curl #2955
    - Separate the code processing currents from MySimulation #2964
    - Add DataConnector::consume(), which shares and consumes the input #2951
    - Move picongpu/simulationControl to picongpu/simulation/control #2971
    - Separate the code processing particles from MySimulation #2974
    - Refactor cell types #2972
    - Rename `compileTime` into `meta` #2983
    - Move fields/FieldManipulator to fields/absorber/ExponentialDamping #2995
    - Add picongpu::particles::manipulate() as a high-level interface to particle manipulation #2993
    - `particles::forEach` #2991
    - Refactor and modernize implementation of fields #3005
    - Modernize ArgsParser::ArgsErrorCode #3023
    - Allow constructor for density free formular functor #3024
    - Reduce PML memory consumption #3122
    - Bremsstrahlung: use more constexpr #3176
    - Pass mapping description by value instead of pointer from simulation stages #3014
    - Add missing inline specifiers for functions defined in header files #3051
    - Remove ZigZag current deposition #2837
    - Fix style issues with particlePusherAcceleration #2781
  - PMacc:

        * Supercell particle counter #2637
        * ForEachIdx::operator(): Use Universal Reference #2881
        * Remove duplicated definition of `BOOST_MPL_LIMIT_VECTOR_SIZE` #2883
        * Cleanup `pmacc/types.hpp` #2927
        * Add pmacc::memory::makeUnique similar to std::make_unique #2949
        * PMacc Vector: C++11 Using #2957
        * Remove pmacc::forward and pmacc::RefWrapper #2963
        * Add const getters to ParticleBox #2941
        * Remove unused pmacc::traits::GetEmptyDefaultConstructibleType #2976
        * Remove pmacc::traits::IsSameType which is no longer used #2979
        * Remove template parameter for initialization method of Pointer and FramePointer #2977
        * Remove pmacc::expressions which is no longer used #2978
        * Remove unused pmacc::IDataSorter #3030
        * Change PMACC_C_STRING to produce a static constexpr member #3050
        * Refactor internals of pmacc::traits::GetUniqueTypeId #3049
        * rename "counterParticles" to "numParticles" #3062
        * Make pmacc::DataSpace conversions explicit #3124
    - plugins:
        * Small update for python visualizers #2882
        * Add namespace "radiation" around code related to radiation plugin #3004
        * Remove unused includes of pthread #3040
        * SpeciesEligibleForSolver for radiation plugin #3061
        * ADIOS: Avoid unsafe temporary strings #2946
    - tools:
        * Update cuda_memtest: CMake CUDA_ROOT Env #2892
        * Update hemera tpl after SLURM update #3123
    - Add pillow as dependency #3180
    - Params: remove `boost::vector<>` usage #2769
    - Use _X syntax in OnceIonized manipulator #2745
    - Add missing const to some GridController getters #3154
- documentation:
    - Containers: Update 0.4.0 #2750
    - Merge 0.4.0 Changelog #2748
    - Update Readme & License: People #2749
    - Add .zenodo.json #2747
    - Fix species.param docu (in all examples too) #2795
    - Fix species.param example doc and grammar #2793
    - Further improve wording in docs #2710
    - MemoryCalculator: fix example output for documentation #2822

- Manual: Plugin & Particle Sections, Map #2820
- System: D.A.V.I.D.E #2821
- License Header: Update 2019 #2845
- Docs: Memory per Device Spelling #2868
- CMake 3.11.0+ #2959
- CUDA 9.0+, GCC 5.1+, Boost 1.65.1+ #2961
- CMake: CUDA 9.0+ #2965
- Docs: Update Sphinx #2969
- CMake: CUDA 9.2-10.1, Boost <= 1.70.0 #2975
- Badge: Commits Since Release & Good First #2980
- Update info on maintainers in README.md #2984
- Fix grammar in all `.profile.example` #2930
- Docs: Dr.s #3009
- Fix old file name in radiation doc #3018
- System: ARIS #3039
- fix typo in getNode and getDevice #3046
- Window move point clean up #3045
- Docs: Cori's KNL Nodes (NERSC) #3043
- Fix various sphinx issues not related to doxygen #3056
- Extend the particle merger plugin documentation #3057
- Fix docs using outdated ManipulateDeriveSpecies #3068
- Adjust cores per gpu on taurus after multicore update #3071
- Docs: create conda env for building docs #3074
- Docs: add missing checkpoint options #3080
- Remove titan ornl setup and doc #3086
- Summit: Profile & Templates #3007
- Update URL to ADIOS #3099
- License Header: Update 2020 #3138
- Add PhD thesis reference in radiation plugin #3151
- Spack: w/o Modules by Default #3182
- Add a brief description of simulation output to basics #3183
- Fix a typo in exchange communication tag status output #3141
- Add a link to PoGit to the docs #3115
- fix optional install instructions in the Summit profile #3094
- Update the form factor documentation #3083
- Docs: Add New References #3072
- Add information about submit.cfg and submit.tpl files to docs. #3070
- Fix style (underline length) in profile.rst #2936
- Profiles: Section Title Length #2934

  - Contributor name typo in LICENSE.md #2880
  - Update modules and memory in gpu_picongpu.profile #2923
  - Add k80_picongpu.profile and k80.tpl #2919
  - Update taurus-tud profiles for the `ml` partition #2903
  - Hypnos: CMake 3.13.4 #2887
  - Docs: Install Blosc #2829
  - Docs: Source Intro Details #2828
  - Taurus Profile: Project #2819
  - Doc: Add System Links #2818
  - remove grep file redirect #2788
  - Correct jupyter widget example #3191
  - fix typo: `UNIT_LENGHT` to `UNIT_LENGTH` #3194
  - Change link to CRP group @ HZDR #2814
- Examples: Unify .cfg #2826
- Remove unused ABSORBER_FADE_IN_STEPS from .param files in examples #2942
- Field absorber test example #2948
- Singularity: Avoid Dotfiles in Home #2981
- Boost: No std::auto_ptr #3012
- Add YeePML to comments for field solver selection #3042
- Add a runtime parameter for window move point #3022
- Ionization: add silicon to pre-defines #3078
- Add 1.cfg to Bremsstrahlung example #3098
- Fix cmake flags for MSVS #3126
- Fix missing override flags #3156
- Fix warning #222-D: floating-point operation result is out of range #3170
- Update alpaka to 0.4.0 and cupla to 0.2.0 #3175
- Slurm update taurus: workdir to chdir #3181
- Adjust profiles for taurus-tud #2990
- Update mallocMC to 2.3.1crp #2893
- Change imread import from scipy.misc to imageio #3192

1.5.3 0.4.3

Date: 2019-02-14

System Updates and Bug Fixes

This release adds updates and new HPC system templates. Important bug fixes include I/O work-arounds for issues in OpenMPI 2.0-4.0 (mainly with HDF5), guards for particle creation with user-defined profiles, a fixed binomial current smoothing, checks for the number of devices in grid distributions and container (Docker & Singularity) modernizations.

Thanks to Axel Huebl, Alexander Debus, Igor Andriyash, Marco Garten, Sergei Bastrakov, Adam Simpson, Richard Pausch, Juncheng E, Klaus Steiniger, and René Widera for contributions to this release!

Changes to "0.4.2"

Bug Fixes:

- fix particle creation if density <= zero #2831
- fix binomial current interpolation #2838
- Docker & Singularity updates #2847
- OpenMPI: use ROMIO for IO #2841 #2857
- `--gridDist`: verify devices and blocks #2876
- Phase space plugin: unit of colorbar in 2D3V #2878

Misc:

- `ionizer.param`: fix typo in "Aluminium" #2865
- System Template Updates:
  - Add system links #2818
  - Taurus:
    - add project #2819
    - add Power9 V100 nodes #2856
  - add D.A.V.I.D.E (CINECA) #2821
  - add JURECA (JSC) #2869
  - add JUWELS (JSC) #2874
  - Hypnos (HZDR): CMake update #2887
  - Slurm systems: link `stdout` to `simOutput/output` #2839
- Docs:
  - Change link to CRP group @ HZDR #2814
  - `FreeRng.def`: typo in example usage #2825
  - More details on source builds #2828
  - Dependencies: Blosc install #2829
  - Ionization plot title linebreak #2867
- plugins:
  - ADIOS & phase space `-Wterminate` #2817
  - Radiation: update documented options #2842
- Update versions script: containers #2846
- pyflakes: `str`/`bytes`/`int` compares #2866
- Travis CI: Fix Spack CMake Install #2879
- Contributor name typo in `LICENSE.md` #2880
- Update mallocMC to 2.3.1crp #2893
- CMake: Honor `_ROOT` Env Hints #2891 #2892 #2893

1.5.4 0.4.2

Date: 2018-11-19

CPU Plugin Performance

This release fixes a performance regression for energy histograms and phase space plugins on CPU with our OpenMP backend on CPU. At least OpenMP 3.1 is needed to benefit from this. Additionally, several small documentation issues have been fixed and the energy histogram python tool forgot to return the first iteration.

Thanks to Axel Huebl, René Widera, Sebastian Starke, and Marco Garten for contributions to this release!

Changes to "0.4.1"

Bug Fixes:

- Plugin performance regression:
  - Speed of plugins `EnergyHistogram` and `PhaseSpace` on CPU (`omp2b`) #2802
- Tools:
  - Python `EnergyHistogramData`: skip of first iteration #2799

Misc:

- update Alpaka to 0.3.5 to fix #2802
- Docs:
  - CFL Static Assert: new grid.param #2804
  - missing exponent in fieldIonization.rst #2790
  - remove grep file redirect #2788
  - Calorimeter Plugin: Document File Suffix #2800

1.5.5 0.4.1

Date: 2018-11-06

Minor Bugs and Example Updates

This release fixes minor bugs found after the 0.4.0 release. Some examples were slightly outdated in syntax, the new "probe particle" `EveryNthCell` initialization functor was broken when not used with equal spacing per dimension. In some rare cases, sliding could occur twice in moving window simulations.

Thanks to Axel Huebl, René Widera, Richard Pausch and Andrei Berceanu for contributions to this release!

Changes to "0.4.0"

Bug Fixes:

- PIConGPU:
  - avoid sliding twice in some corner-cases #2774
  - EveryNthCell: broken if not used with same spacing #2768
  - broken compile with particle merging #2753
- Examples:
  - fix outdated derive species #2756
  - remove current deposition in bunch example #2758

  - fix 2D case of single electron init (via density) #2766
- Tools:
  - Python Regex: r Literals #2767
  - `cuda_memtest`: avoid noisy output if NVML is not found #2785

Misc:

- `.param` files: refactor `boost::vector<>` usage #2769
- Docs:
  - Spack: Improve Bootstrap #2773
  - Fix docs for radiation in 2D #2772
  - Containers: Update 0.4.0 #2750
  - Update Readme & License: People #2749
  - Add `.zenodo.json` #2747

1.5.6 0.4.0

Date: 2018-10-19

CPU Support, Particle Filter, Probes & Merging

This release adds CPU support, making PIConGPU a many-core, single-source, performance portable PIC code for all kinds of supercomputers. We added particle filters to initialization routines and plugins, allowing fine-grained in situ control of physical observables. All particle plugins now support those filters and can be called multiple times with different settings.

Particle probes and more particle initialization manipulators have been added. A particle merging plugin has been added. The Thomas-Fermi model has been improved, allowing to set empirical cut-offs. PIConGPU input and output (plugins) received initial Python bindings for efficient control and analysis.

User input files have been dramatically simplified. For example, creating the PIConGPU binary from input files for GPU or CPU is now as easy as `pic-build -b cuda` or `pic-build -b omp2b` respectively.

Thanks to Axel Huebl, René Widera, Benjamin Worpitz, Sebastian Starke, Marco Garten, Richard Pausch, Alexander Matthes, Sergei Bastrakov, Heiko Burau, Alexander Debus, Ilja Göthel, Sophie Rudat, Jeffrey Kelling, Klaus Steiniger, and Sebastian Hahn for contributing to this release!

Changes to "0.3.0"

User Input Changes:

- (re)move directory `simulation_defines/` #2331
- add new param file `particleFilters.param` #2385
- `components.param`: remove define `ENABLE_CURRENT` #2678
- `laser.param`: refactor Laser Profiles to Functors #2587 #2652
- `visualization.param`: renamed to `png.param` #2530
- `speciesAttributes.param`: format #2087
- `fieldSolver.param`: doxygen, refactored #2534 #2632
- `mallocMC.param`: file doxygen #2594
- `precision.param`: file doxygen #2593
- `memory.param`:

  - `GUARD_SIZE` docs #2591
  - exchange buffer size per species #2290
  - guard size per dimension #2621
- `density.param`:
  - Gaussian density #2214
  - Free density: fix `float_X` #2555
- `ionizer.param`: fixed excess 5p shell entry in gold effective Z #2558
- `seed.param`:
  - renamed to `random.param` #2605
  - expose random number method #2605
- `isaac.param`: doxygen documentation #2260
- `unit.param`:
  - doxygen documentation #2467
  - move conversion units #2457
  - earlier normalized speed of light in `physicalConstants.param` #2663
- `float_X` constants to literals #2625
- refactor particle manipulators #2125
- new tools:
  - `pic-edit`: adjust `.param` files #2219
  - `pic-build`: combine pic-configure and make install #2204
- `pic-configure`:
  - select CPU/GPU backend and architecture with `-b` #2243
  - default backend: CUDA #2248
- `tbg`:
  - `.tpl` no `_profile` suffix #2244
  - refactor `.cfg` files: devices #2543
  - adjust LWFA setup for 8GPUs #2480
- `SliceField` plugin: Option `.frequency` to `.period`#2034
- particle filters:
  - add filter support to phase space plugin #2425
  - multi plugin energy histogram with filter #2424
  - add particle filter to `EnergyParticles` #2386
- Default Inputs: C++11 `using` for `typedef` #2315
- Examples: C++11 `using` for `typedef` #2314
- Python: Parameter Ranges for Param Files (LWFA) #2289
- `FieldTmp`: `SpeciesEligibleForSolver` Traits #2377
- Particle Init Methods: Unify API & Docs #2442
- get species by name #2464
- remove template dimension from current interpolator's #2491

- compile time string #2532

New Features:

- PIC:
  - particle merging #1959
  - check cells needed for stencils #2257
  - exchange buffer size per species #2290
  - push with `currentStep` #2318
  - `InitController`: unphysical particles #2365
  - New Trait: `SpeciesEligibleForSolver` #2364
  - Add upper energy cut-off to ThomasFermi model #2330
  - Particle Pusher: Probe #2371
  - Add lower ion density cut-off to ThomasFermi model #2361
  - CT Factory: `GenerateSolversIfSpeciesEligible` #2380
  - add new param file `particleFilters.param` #2385
  - Probe Particle Usage #2384
  - Add lower electron temperature cut-off to ThomasFermi model #2376
  - new particle filters #2418 #2659 #2660 #2682
  - Derived Attribute: Bound Electron Density #2453
  - get species by name #2464
  - New Laser Profile: Exp. Ramps with Prepulse #2352
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  - expose random number method to the user #2605
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  - fix stencil conditions #2613
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    - fix illegal memory access #2151
    - fix possible deadlock in blocking MPI ops #2683
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    - `HostBuffer` 1D Support #2657
  - fix warning concerning forward declarations of `pmacc::detail::Environment` #2489
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  - pic-configure: cmakeFlags return code #2323
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* Restructure Repository Structure #2135
* lockstep refactoring `KernelManipulateAllParticles` #2140
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* improve speed to calculate number of ppc #2274
* refactor `picongpu::particles::startPosition` #2168
* Particle Pusher: Clean-Up Interface #2359
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* Start Pos: OnePosition w/o Weighting #2378
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* FieldTmp: `SpeciesEligibleForSolver` Traits #2377
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    * refactor PMacc functor interface #2395
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    * lockstep refactoring of `KernelCountParticles` #2061
    * lockstep refactoring `KernelFillGapsLastFrame` #2055
    * lockstep refactoring of `KernelFillGaps` #2083
    * lockstep refactoring of `KernelDeleteParticles` #2084
    * lockstep refactoring of `KernelInsertParticles` #2089
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    * Add a workaround for `PMACC_STRUCT` to work in Visual Studio #2502
    * Fix type of index in OpenMP-parallelized loop #2505
    * add support for CUDA9 `__shfl_snyc, __ballot_sync` #2348
    * Partially replace compound literals in PMacc #2494
    * fix type cast in `pmacc::exec::KernelStarter::operator()` #2518
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    * Png Plugin: Boost to std Thread #2197
    * lockstep kernel refactoring `KernelRadiationParticles` #2240
    * generic multi plugin #2375
    * add particle filter to `EnergyParticles` #2386
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    * lockstep kernel refactoring `ParticleCalorimeter` #2291
    * Splash: 1.7.0 #2520
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    * Tools: All C++11 #2194
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      · better handling of missing egetopt error message #2712
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  - Reduce # photons in Bremsstrahlung example #1979
  - TBG: .tpl no `_profile` suffix #2244
  - Default Inputs: C++11 Using for Typedef #2315
  - Examples: C++11 Using for Typedef #2314
  - LWFA Example: Restore a0=8.0 #2324
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  - PIConGPU use tiny RNG #2447
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  - (Re)Move simulation_defines/ #2331
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  - Params: float_X Constants to Literals #2625
- documentation:
  - new subtitle #2734

- Lockstep Programming Model #2026 #2064
- `IdxConfig` append documentation #2022
- `multiMask`: Refactor Documentation #2119
- `CtxArray` #2390
- Update openPMD Post-Processing #2322 #2733
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- Update EnergyFields #2559
- Note on Energy Reduce #2584
- ADIOS: More Transport & Compression Doc #2640
- ADIOS Metafile #2633
- radiation parameters #1986
- CPU Compile #2185
- `pic-configure` help #2191
- Python yt 3.4 #2273
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- Remove ToDo from `ionizationEnergies.param` #1989
- Parameter Order in Manual #1991
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  - Document Laser Cutoff #2000
  - Move Author Macros #2005
  - PDF Radiation #2184
  - Changelog in Manual #2527
- PBS usage example #2006
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- fix spelling of guard #2644
- param: extended description #2041
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- Dev Version: 0.4.0-dev #2085
- Fix typo in ADK documentation #2096
- Profile Preparations #2095
- SuperConfig: Header Fix #2108
- Extended $SCRATCH Info #2093
- Doxygen: Fix Headers #2118
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- CMake 3.7.0 #2181
- Boost (1.62.0-) 1.65.1 - 1.68.0 #2182 #2707 #2713
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- Install Docs: CUDA is optional #2199
- Fix broken links #2200
- PIConGPU Logo: More Platforms #2190
- Repo Structure #2218
- Document KNL GCC -march #2252
- Streamline Install #2256
- Added doxygen documentation for isaac.param file #2260
- License Docs: Update #2282
- Heiko to Former Members #2294
- Added an example profile and tpl file for taurus' KNL #2270
- Profile: Draco (MPCDF) #2308
- $PIC_EXAMPLES #2327
- Profiles for Titan & Taurus #2201
- Taurus:
  * CUDA 8.0.61 #2337
  * Link KNL Profile #2339
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- Move ParaView Profile #2353
- Spack: Own GitHub Org #2358
- LWFA Example: Improve Ranges #2360
- fix spelling mistake in checkpoint #2372
- Spack Install: Clarify #2373 #2720
- Probe Pusher #2379
- CI/Deps: CUDA 8.0 #2420
- Piz Daint (CSCS):
  * Update Profiles #2306 #2655

        * ADIOS Build #2343
        * ADIOS 1.13.0 #2416
        * Update CMake #2436
        * Module Update #2536
        * avoid `pmi_alps` warnings #2581
    - Hypnos (HZDR): New Modules #2521 #2661
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    - Hypnos & Taurus: Profile Examples Per Queue #2249
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    - Community Map #2445
    - License Header: Update 2018 #2448
    - Docker: Nvidia-Docker 2.0 #2462 #2557
    - Hide Double ToC #2463
    - Param Docs: Title Only #2466
    - New Developers #2487
    - Fix Docs: `FreeTotalCellOffset` Filter #2493
    - Stream-line Intro #2519
    - Fix HDF5 Release Link #2544
    - Minor Formatting #2553
    - PIC Model #2560
    - Doxygen: Publish As Well #2575
    - Limit Filters to Eligible Species #2574
    - Doxygen: Less XML #2641
    - NVCC 8.0 GCC <= 5.3 && 9.0/9.1: GCC <= 5.5 #2639
    - typo: element-wise #2638
    - fieldSolver.param doxygen #2632
    - `memory.param`: `GUARD_SIZE` docs #2591
    - changelog script updated to python3 #2646
- not yet supported on CPU (Alpaka): #2180
    - core:
        * Bremsstrahlung
    - plugins:
        * PositionsParticles
        * ChargeConservation
        * ParticleMerging
        * count per supercell (macro particles)
        * field intensity

1.5.7 0.3.2

Date: 2018-02-16

Phase Space Momentum, ADIOS One-Particle Dumps & Field Names

This release fixes a bug in the phase space plugin which derived a too-low momentum bin for particles below the typical weighting (and too-high for above it). ADIOS dumps crashed on one-particle dumps and in the name of on-the-fly particle-derived fields species name and field name were in the wrong order. The plugins libSplash (1.6.0) and PNGwriter (0.6.0) need exact versions, later releases will require a newer version of PIConGPU.

Changes to "0.3.1"

Bug Fixes:

- PIConGPU:
  - wrong border with current background field #2326
- libPMacc:
  - cuSTL: missing include in `ForEach` #2406
  - warning concerning forward declarations of `pmacc::detail::Environment` #2489
  - `pmacc::math::Size_t<0>::create()` in Visual Studio #2513
- plugins:
  - phase space plugin: weighted particles' momentum #2428
  - calorimeter: validate `minEnergy` #2512
  - ADIOS:
    - one-particle dumps #2437
    - `FieldTmp`: derived field name #2461
  - exact versions of libSplash 1.6.0 & PNGwriter 0.6.0
- tools:
  - tbg: wrong quoting of `'` #2419
  - CMake: false-positive on in-source build check #2407
  - pic-configure: cmakeFlags return code #2323

Misc:

- Hypnos (HZDR): new modules #2521 #2524

Thanks to Axel Huebl, René Widera, Sergei Bastrakov and Sebastian Hahn for contributing to this release!

1.5.8 0.3.1

Date: 2017-10-20

Field Energy Plugin, Gaussian Density Profile and Restarts

This release fixes the energy field plugin diagnostics and the "downramp" parameter of the pre-defined Gaussian density profile. Restarts with enabled background fields were fixed. Numerous improvements to our build system were added to deal more gracefully with co-existing system-wide default libraries. A stability issue due to an illegal memory access in the PMacc event system was fixed.

Changes to "0.3.0"

.param file changes:

- `density.param`: in `Gaussian` profile, the parameter `gasSigmaRight` was not properly honored but `gasCenterRight` was taken instead #2214
- `fieldBackground.param`: remove micro meters usage in default file #2138

Bug Fixes:

- PIConGPU:
  - `gasSigmaRight` of `Gaussian` density profile was broken since 0.2.0 release #2214
  - restart with enabled background fields #2113 #2139
  - KHI example: missing constexpr in input #2309
- libPMacc:
  - event system: illegal memory access #2151
- plugins:
  - energy field reduce #2112
- tools:
  - CMake:
    - Boost dependency:
      - same minimal version for tools #2293
      - transient dependenciens: `date_time`, `chrono`, `atomic` #2195
    - use targets of boost & zlib #2193 #2292
    - possible linker error #2107
  - XDMF script: positionOffset for openPMD #2309
  - cmakeFlags: escape lists #2183
  - tbg:
    - `--help` exit with 0 return code #2213
    - env variables: proper handling of \ and & #2262

Misc:

- PIConGPU: `--help` to stdout #2148
- tools: all to C++11 #2194
- documentation:
  - Hypnos .tpl files: remove passing `LD_LIBRARY_PATH` to avoid warning #2149
  - fix plasma frequency and remove German comment #2110
  - remove micro meters usage in default background field #2138
  - README: update links of docs badge #2144

Thanks to Axel Huebl, Richard Pausch and René Widera for contributions to this release!

1.5.9 0.3.0

Date: 2017-06-16

C++11: Bremsstrahlung, EmZ, Thomas-Fermi, Improved Lasers

This is the first release of PIConGPU requiring C++11. We added a newly developed current solver (EmZ), support for the generation of Bremsstrahlung, Thomas-Fermi Ionization, Laguerre-modes in the Gaussian-Beam laser, in-simulation plane for laser initialization, new plugins for in situ visualization (ISAAC), a generalized particle calorimeter and a GPU resource monitor. Initial support for clang (host and device) has been added and our documentation has been streamlined to use Sphinx from now on.

Changes to "0.2.0"

.param & .unitless file changes:

- use C++11 `constexpr` where possible and update arrays #1799 #1909
- use C++11 `using` instead of `typedef`
- removed `Config` suffix in file names #1965
- `gasConfig` is now `density`
- `speciesDefinition`:
  - simplified `Particles<>` interface #1711 #1942
  - `ionizer< ... >` became a sequence of `ionizers< ... >` #1999
- `radiation`: replace `#defines` with clean C++ #1877 #1930 #1931 #1937

Basic Usage:

We renamed the default tools to create, setup and build a simulation. Please make sure to update your `picongpu.profile` with the latest syntax (e.g. new entries in `PATH`) and use from now on:

- `$PICSRC/createParameterSet` -> `pic-create`
- `$PICSRC/configure` -> `pic-configure`
- `$PICSRC/compile` -> `pic-compile`

See the *Installation* and *Usage* chapters in our new documentation on https://picongpu.readthedocs.io for detailed instructions.

New Features:

- PIConGPU:
  - laser:
    - allow to define the initialization plane #1796
    - add transverse Laguerre-modes to standard Gaussian Beam #1580
  - ionization:
    - Thomas-Fermi impact ionization model #1754 #2003 #2007 #2037 #2046
    - Z_eff, energies, isotope: Ag, He, C, O, Al, Cu #1804 #1860
    - BSI models restructured #2013
    - multiple ionization algorithms can be applied per species, e.g. cut-off barrier suppression ionization (BSI), probabilistic field ionization (ADK) and collisional ionization #1999
  - Add EmZ current deposition solver #1582
  - FieldTmp:
    - Multiple slots #1703

        * Gather support to fill GUARD #2009
    - Particle `StartPosition`: `OnePosition` #1753
    - Add Bremsstrahlung #1504
    - Add kinetic energy algorithm #1744
    - Added species manipulators:
        * `CopyAttribute` #1861
        * `FreeRngImpl` #1866
    - Clang compatible static assert usage #1911
    - Use `PMACC_ASSERT` and `PMACC_VERIFY` #1662
- PMacc:
    - Improve PMacc testsystem #1589
    - Add test for IdProvider #1590
    - Specialize HasFlag and GetFlagType for Particle #1604
    - Add generic atomicAdd #1606
    - Add tests for all RNG generators #1494
    - Extent function `twistVectorFieldAxes<>()` #1568
    - Expression validation/assertion #1578
    - Use PMacc assert and verify #1661
    - GetNComponents: improve error message #1670
    - Define `MakeSeq_t` #1708
    - Add `Array<>` with static size #1725
    - Add shared memory allocator #1726
    - Explicit cast `blockIdx` and `threadIdx` to `dim3` #1742
    - CMake: allow definition of multiple architectures #1729
    - Add trait `FilterByIdentifier` #1859
    - Add CompileTime Accessor: Type #1998
- plugins:
    - HDF5/ADIOS:
        * MacroParticleCounter #1788
        * Restart: Allow disabling of moving window #1668
        * FieldTmp: MidCurrentDensityComponent #1561
    - Radiation:
        * Add pow compile time using c++11 #1653
        * Add radiation form factor for spherical Gaussian charge distribution #1641
    - Calorimeter: generalize (charged & uncharged) #1746
    - PNG: help message if dependency is not compiled #1702
    - Added:
        * In situ: ISAAC Plugin #1474 #1630
        * Resource log plugin #1457

- tools:
  - Add a tpl file for k80 hypnos that automatically restarts #1567
  - Python3 compatibility for plotNumericalHeating #1747
  - Tpl: Variable Profile #1975
  - Plot heating & charge conservation: file export #1637
- Support for clang as host && device compiler #1933

Bug Fixes:

- PIConGPU:
  - 3D3V: missing absorber in z #2042
  - Add missing minus sign wavepacket laser transversal #1722
  - `RatioWeighting` (`DensityWeighting`) manipulator #1759
  - `MovingWindow`: `slide_point` now can be set to zero. #1783
  - `boundElectrons`: non-weighted attribute #1808
  - Verify number of ionization energy levels == proton number #1809
  - Ionization:
    - charge of ionized ions #1844
    - ADK: fix effective principal quantum number `nEff` #2011
  - Particle manipulators: position offset #1852
- PMacc:
  - Avoid CUDA local memory usage of `Particle<>` #1579
  - Event system deadlock on `MPI_Barrier` #1659
  - ICC: `AllCombinations` #1646
  - Device selection: guard valid range #1665
  - `MapTuple`: broken compile with icc #1648
  - Missing '%%' to use ptx special register #1737
  - `ConstVector`: check arguments init full length #1803
  - `CudaEvent`: cyclic include #1836
  - Add missing `HDINLINE` #1825
  - Remove `BOOST_BIND_NO_PLACEHOLDERS` #1849
  - Remove CUDA native static shared memory #1929
- plugins:
  - Write openPMD meta data without species #1718
  - openPMD: iterationFormat only Basename #1751
  - ADIOS trait for `bool` #1756
  - Adjust `radAmplitude` python module after openPMD changes #1885
  - HDF5/ADIOS: ill-placed helper `#include` #1846
  - `#include`: never inside namespace #1835
- work-around for bug in boost 1.64.0 (odeint) + CUDA NVCC 7.5 & 8.0 #2053 #2076

Misc:

- refactoring:
  - PIConGPU:
    - Switch to C++11 only #1649
    - Begin kernel names with upper case letter #1691
    - Maxwell solver, use curl instance #1714
    - Lehe solver: optimize performance #1715
    - Simplify species definition #1711
    - Add missing `math::` namespace to `tan()` #1740
    - Remove usage of pmacc and boost auto #1743
    - Add missing `typenames` #1741
    - Change ternary if operator to `if` condition #1748
    - Remove usage of `BOOST_AUTO` and `PMACC_AUTO` #1749
    - mallocMC: organize setting #1779
    - `ParticlesBase` allocate member memory #1791
    - `Particle` constructor interface #1792
    - Species can omit a current solver #1794
    - Use constexpr for arrays in `gridConfig.param` #1799
    - Update mallocMC #1798
    - `DataConnector`: `#includes` #1800
    - Improve Esirkepov speed #1797
    - Ionization Methods: Const-Ness #1824
    - Missing/wrong includes #1858
    - Move functor `Manipulate` to separate file #1863
    - Manipulator `FreeImpl` #1815
    - Ionization: clean up params #1855
    - MySimulation: remove particleStorage #1881
    - New `DataConnector` for fields (& species) #1887 #2045
    - Radiation filter functor: remove macros #1877
    - Topic use remove shared keyword #1727
    - Remove define `ENABLE_RADIATION` #1931
    - Optimize `AssignedTrilinearInterpolation` #1936
    - `Particles<>` interface #1942
    - Param/Unitless files: remove “config” suffix #1965
    - Kernels: Refactor Functions to Functors #1669
    - Gamma calculation #1857
    - Include order in defaut loader #1864
    - Remove `ENABLE_ELECTRONS/IONS` #1935
    - Add `Line<>` default constructor #1588
  - PMacc:

    - Particles exchange: avoid message spamming #1581
    - Change minimum CMake version #1591
    - CMake: handle PMacc as separate library #1692
    - ForEach: remove boost preprocessor #1719
    - Refactor `InheritLinearly` #1647
    - Add missing `HDINLINE` prefix #1739
    - Refactor .h files to .hpp files #1785
    - Log: make events own level #1812
    - float to int cast warnings #1819
    - DataSpaceOperations: Simplify Formula #1805
    - DataConnector: Shared Pointer Storage #1801
    - Refactor `MPIReduce` #1888
    - Environment refactoring #1890
    - Refactor `MallocMCBuffer` share #1964
    - Rename `typedefs` inside `ParticleBuffer` #1577
    - Add typedefs for `Host/DeviceBuffer` #1595
    - DeviceBufferIntern: fix shadowed member variable #2051
  - plugins:
    - Source files: remove non-ASCII chars #1684
    - replace old analyzer naming #1924
    - Radiation:
      - Remove Nyquist limit switch #1930
      - Remove precompiler flag for form factor #1937
    - compile-time warning in 2D live plugin #2063
  - tools:
    - Automatically restart from ADIOS output #1882
    - Workflow: rename tools to set up a sim #1971
    - Check if binary `cuda_memtest` exists #1897
  - C++11 constexpr: remove boost macros #1655
  - Cleanup: remove EOL white spaces #1682
  - .cfg files: remove EOL white spaces #1690
  - Style: more EOL #1695
  - Test: remove more EOL white spaces #1685
  - Style: replace all tabs with spaces #1698
  - Pre-compiler spaces #1693
  - Param: Type List Syntax #1709
  - Refactor Density Profiles #1762
  - Bunch Example: Add Single e- Setup #1755
  - Use Travis `TRAVIS_PULL_REQUEST_SLUG` #1773

  - ManipulateDeriveSpecies: Refactor Functors & Tests #1761
  - Source Files: Move to Headers #1781
  - Single Particle Tests: Use Standard MySimulation #1716
  - Replace NULL with C++11 nullptr #1790
- documentation:
  - Wrong comment random->quiet #1633
  - Remove `sm_20` Comments #1664
  - Empty Example & `TBG_macros.cfg` #1724
  - License Header: Update 2017 #1733
  - speciesInitialization: remove extra typename in doc #2044
  - INSTALL.md:
    - List Spack Packages #1764
    - Update Hypnos Example #1807
    - grammar error #1941
  - TBG: Outdated Header #1806
  - Wrong sign of `delta_angle` in radiation observer direction #1811
  - Hypnos: Use CMake 3.7 #1823
  - Piz Daint: Update example environment #2030
  - Doxygen:
    - Warnings Radiation #1840
    - Warnings Ionization #1839
    - Warnings PMacc #1838
    - Warnings Core #1837
    - Floating Docstrings #1856
    - Update `struct.hpp` #1879
    - Update FieldTmp Operations #1789
    - File Comments in Ionization #1842
    - Copyright Header is no Doxygen #1841
  - Sphinx:
    - Introduce Sphinx + Breathe + Doxygen #1843
    - PDF, Link rst/md, png #1944 #1948
    - Examples #1851 #1870 #1878
    - Models, PostProcessing #1921 #1923
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    - Local Build Instructions #1922
    - Python Tutorials #1872
    - Core Param Files #1869
    - Important Classes #1871
    - .md files, tbg, profiles #1883

        - `ForEach` & Identifier #1889
        - References & Citation #1895
        - Slurm #1896 #1952
        - Restructure Install Instructions #1943
        - Start a User Workflows Section #1955
    - ReadTheDocs:
        - Build PDF & EPUB #1947
        - remove linenumbers #1974
    - Changelog & Version 0.2.3 (master) #1847
    - Comments and definition of `radiationObserver` default setup #1829
    - Typos plot radiation tool #1853
    - doc/ -> docs/ #1862
    - Particles Init & Manipulators #1880
    - INSTALL: Remove gimli #1884
    - BibTex: Change ShortHand #1902
    - Rename `slide_point` to `movePoint` #1917
    - Shared memory allocator documenation #1928
    - Add documentation on slurm job control #1945
    - Typos, modules #1949
    - Mention current solver `EmZ` and compile tests #1966
- Remove assert.hpp in radiation plugin #1667
- Checker script for `__global__` keyword #1672
- Compile suite: GCC 4.9.4 chain #1689
- Add TSC and PCS rad form factor shapes #1671
- Add amend option for tee in k80 autorestart tpl #1681
- Test: EOL and suggest solution #1696
- Test: check & remove pre-compiler spaces #1694
- Test: check & remove tabs #1697
- Travis: check PR destination #1732
- Travis: simple style checks #1675
- PositionFilter: remove (virtual) Destructor #1778
- Remove namespace workaround #1640
- Add Bremsstrahlung example #1818
- WarmCopper example: FLYlite benchmark #1821
- Add compile tests for radiation methods #1932
- Add visual studio code files to gitignore #1946
- Remove old QT in situ volume visualization #1735

Thanks to Axel Huebl, René Widera, Alexander Matthes, Richard Pausch, Alexander Grund, Heiko Burau, Marco Garten, Alexander Debus, Erik Zenker, Bifeng Lei and Klaus Steiniger for contributions to this release!

1.5.10 0.2.5

Date: 2017-05-27

Absorber in z in 3D3V, effective charge in ADK ionization

The absorbing boundary conditions for fields in 3D3V simulations were not enabled in z direction. This caused unintended reflections of electro-magnetic fields in z since the 0.1.0 (beta) release. ADK ionization was fixed to the correct charge state (principal quantum number) which caused wrong ionization rates for all elements but Hydrogen.

Changes to "0.2.5"

Bug Fixes:

- ADK ionization: effective principal quantum number nEff #2011
- 3D3V: missing absorber in z #2042

Misc:

- compile-time warning in 2D live plugin #2063
- DeviceBufferIntern: fix shadowed member variable #2051
- speciesInitialization: remove extra typename in doc #2044

Thanks to Marco Garten, Richard Pausch, René Widera and Axel Huebl for spotting the issues and providing fixes!

1.5.11 0.2.4

Date: 2017-03-06

Charge of Bound Electrons, openPMD Axis Range, Manipulate by Position

This release fixes a severe bug overestimating the charge of ions when used with the `boundElectrons` attribute for field ionization. For HDF5 & ADIOS output, the openPMD axis annotation for fields in simulations with non-cubic cells or moving window was interchanged. Assigning particle manipulators within a position selection was rounded to the closest supercell (`IfRelativeGlobalPositionImpl`).

Changes to "0.2.3"

Bug Fixes:

- ionization: charge of ions with `boundElectrons` attribute #1844
- particle manipulators: position offset, e.g. in `IfRelativeGlobalPositionImpl` rounded to supercell #1852 #1910
- PMacc:
  - remove `BOOST_BIND_NO_PLACEHOLDERS` #1849
  - add missing `HDINLINE` #1825
  - `CudaEvent`: cyclic include #1836
- plugins:
  - std includes: never inside namespaces #1835
  - HDF5/ADIOS openPMD:
    - GridSpacing, GlobalOffset #1900
    - ill-places helper includes #1846

Thanks to Axel Huebl, René Widera, Thomas Kluge, Richard Pausch and Rémi Lehe for spotting the issues and providing fixes!

1.5.12 0.2.3

Date: 2017-02-14

Energy Density, Ionization NaNs and openPMD

This release fixes energy density output, minor openPMD issues, corrects a broken species manipulator to derive density weighted particle distributions, fixes a rounding issue in ionization routines that can cause simulation corruption for very small particle weightings and allows the moving window to start immediately with timestep zero. For ionization input, we now verify that the number of arguments in the input table matches the ion species' proton number.

Changes to "0.2.2"

Bug Fixes:

- openPMD:
  - iterationFormat only basename #1751
  - ADIOS trait for bool #1756
  - boundElectrons: non-weighted attribute #1808
- RatioWeighting (DensityWeighting) manipulator #1759
- MovingWindow: slide_point now can be set to zero #1783
- energy density #1750 #1744 (partial)
- possible NAN momenta in ionization #1817
- `tbg` bash templates were outdated/broken #1831

Misc:

- ConstVector:
  - check arguments init full length #1803
  - float to int cast warnings #1819
- verify number of ionization energy levels == proton number #1809

Thanks to Axel Huebl, René Widera, Richard Pausch, Alexander Debus, Marco Garten, Heiko Burau and Thomas Kluge for spotting the issues and providing fixes!

1.5.13 0.2.2

Date: 2017-01-04

Laser wavepacket, vacuum openPMD & icc

This release fixes a broken laser profile (wavepacket), allows to use icc as the host compiler, fixes a bug when writing openPMD files in simulations without particle species ("vacuum") and a problem with GPU device selection on shared node usage via `CUDA_VISIBLE_DEVICES`.

Changes to "0.2.1"

Bug Fixes:

- add missing minus sign wavepacket laser transversal #1722
- write openPMD meta data without species #1718
- device selection: guard valid range #1665
- PMacc icc compatibility:
  - `MapTuple` #1648
  - `AllCombinations` #1646

Misc:

- refactor `InheritLinearly` #1647

Thanks to René Widera and Richard Pausch for spotting the issues and providing fixes!

1.5.14 0.2.1

Date: 2016-11-29

QED synchrotron photon & fix potential deadlock in checkpoints

This releases fixes a potential deadlock encountered during checkpoints and initialization. Furthermore, we forgot to highlight that the 0.2.0 release also included a QED synchrotron emission scheme (based on the review in A. Gonoskov et al., PRE 92, 2015).

Changes to "0.2.0"

Bug Fixes:

- potential event system deadlock init/checkpoints #1659

Thank you to René Widera for spotting & fixing and Heiko Burau for the QED synchrotron photon emission implementation!

1.5.15 0.2.0 "Beta"

Date: 2016-11-24

Beta release: full multiple species support & openPMD

This release of PIConGPU, providing "beta" status for users, implements full multi-species support for an arbitrary number of particle species and refactors our main I/O to be formatted as openPMD (see http://openPMD.org). Several major features have been implemented and stabilized, highlights include refactored ADIOS support (including checkpoints), a classical radiation reaction pusher (based on the work of M. Vranic/IST), parallel particle-IDs, generalized on-the-fly particle creation, advanced field ionization schemes and unification of plugin and file names.

This is our last C++98 compatible release (for CUDA 5.5-7.0). Upcoming releases will be C++11 only (CUDA 7.5+), which is already supported in this release, too.

Thank you to Axel Huebl, René Widera, Alexander Grund, Richard Pausch, Heiko Burau, Alexander Debus, Marco Garten, Benjamin Worpitz, Erik Zenker, Frank Winkler, Carlchristian Eckert, Stefan Tietze, Benjamin Schneider, Maximilian Knespel and Michael Bussmann for contributions to this release!

Changes to "0.1.0"

Input file changes: the generalized versions of input files are as always in `src/picongpu/include/simulation_defines/`.

.param file changes:

- all `const` parameters are now `BOOST_CONSTEXPR_OR_CONST`
- add pusher with radiation reaction (Reduced Landau Lifshitz) #1216
- add manipulator for setting `boundElectrons<>` attribute #768
- add `PMACC_CONST_VECTOR` for ionization energies #768 #1022
- `ionizationEnergies.param` #865
- `speciesAttributes.param`: add ionization model `ADK` (Ammosov-Delone-Krainov) for lin. pol. and circ. pol cases #922 #1541
- `speciesAttributes.param`: rename `BSI` to `BSIHydrogenLike`, add `BSIStarkShifted` and `BSIEffectiveZ` #1423
- `laserConfig.param`: documentation fixed and clearified #1043 #1232 #1312 #1477
- `speciesAttributes.param`: new required traits for for each attribute #1483
- `species*.param`: refactor species mass/charge definition (relatve to base mass/charge) #948
- `seed.param`: added for random number generator seeds #951
- remove use of native `double` and `float` #984 #991
- `speciesConstants.param`: move magic gamma cutoff value from radition plugin here #713
- remove invalid `typename` #926 #944

.unitless file changes:

- add pusher with radiation reaction (Reduced Landau Lifshitz) #1216
- pusher traits simplified #1515
- fieldSolver: numericalCellType is now a namespace not a class #1319
- remove usage of native `double` and `float` #983 #991
- remove invalid `typename` #926
- add new param file: `synchrotronPhotons.param` #1354
- improve the CFL condition depending on dimension in KHI example #774
- add laserPolynom as option to `componentsConfig.param` #772

tbg: template syntax

Please be aware that templates (`.tpl`) used by `tbg` for job submission changed slightly. Simply use the new system-wise templates from `src/picongpu/submit/`. #695 #1609 #1618

Due to unifications in our command line options (plugins) and multi-species support, please update your `.cfg` files with the new namings. Please visit `doc/TBG_macros.cfg` and our wiki for examples.

New Features:

- description of 2D3V simulations is now scaled to a user-defined "dZ" depth looking like a one-z-cell 3D simulation #249 #1569 #1601
- current interpolation/smoothing added #888
- add synchrotron radiation of photons from QED- and classical spectrum #1354 #1299 #1398
- species attributes:
  - particle ids for tracking #1410

  - self-describing units and dimensionality #1261
  - add trait `GetDensityRatio`, add attribute `densityRatio`
  - current solver is now a optinal for a species #1228
  - interpolation is now a optional attribute for a species #1229
  - particle pusher is now a optional attribute for a species #1226
  - add species shape piecewise biqudratic spline `P4S` #781
- species initialization:
  - add general particle creation module #1353
  - new manipulators to clone electrons from ions #1018
  - add manipulator to change the in cell position after gas creation #947 #959
  - documentation #961
- species pushers:
  - enable the way for substepping particle pushers as RLL
    - add pusher with radiation reaction (Reduced Landau Lifshitz) #1216
    - enable substepping in pushers #1201 #1215 #1339 #1210 #1202 #1221
    - add Runge Kutta solver #1177
    - enable use of macro-particle weighting in pushers #1213
  - support 2D for all pushers #1126
- refactor gas profile definitions #730 #980 #1265
- extend `FieldToParticleInterpolation` to 1D- and 2D-valued fields #1452
- command line options:
  - parameter validation #863
  - support for `--softRestarts <n>` to loop simulations #1305
  - a simulation `--author` can be specified (I/O, etc.) #1296 #1297
  - calling `./picongpu` without arguments triggers `--help` #1294
- FieldTmp:
  - scalar fields renamed #1259 #1387 #1523
  - momentum over component #1481
- new traits:
  - `GetStringProperties` for all solvers and species flags #1514 #1519
  - `MacroWeighted` and `WeightingPower` #1445
- speedup current deposition solver ZigZag #927
- speedup particle operations with collective atomics #1016
- refactor particle update call #1377
- enable 2D for single particle test #1203
- laser implementations:
  - add phase to all laser implementations #708
  - add in-plane polarization to TWTS laser #852
  - refactor specific float use in laser polynom #782

  - refactored TWTS laser #704
- checkpoints: now self-test if any errors occured before them #897
- plugins:
  - add 2D support for SliceFieldPrinter plugin #845
  - notify plugins on particles leaving simulation #1394
  - png: threaded, less memory hungry in 2D3V, with author information #995 #1076 #1086 #1251 #1281 #1292 #1298 #1311 #1464 #1465
  - openPMD support in I/O
    * HDF5 and ADIOS plugin refactored #1427 #1428 #1430 #1478 #1517 #1520 #1522 #1529
    * more helpers added #1321 #1323 #1518
    * both write now in a sub-directory in simOutput: h5/ and bp/ #1530
    * getUnit and getUnitDimension in all fields & attributes #1429
  - ADIOS:
    * prepare particles on host side befor dumping #907
    * speedup with `OpenMP` #908
    * options to control striping & meta file creation #1062
    * update to 1.10.0+ #1063 #1557
    * checkpoints & restarts implemented #679 #828 #900
  - speedup radioation #996
  - add charge conservation plugin #790
  - add calorimeter plugin #1376
  - radiation:
    * ease restart on command line #866
    * output is now openPMD compatible #737 #1053
    * enable compression for hdf5 output #803
    * refactor specific float use #778
    * refactor radiation window function for 2D/3D #799
- tools:
  - add error when trying to compile picongpu with CUDA 7.5 w/o C++11 #1384
  - add tool to load hdf5 radiation data into python #1332
  - add uncrustify tool (format the code) #767
  - live visualisation client: set fps panal always visible #1240
  - tbg:
    * simplify usage of `-p|--project` #1267
    * transfers UNIX-permisions from `*.tpl` to submit.start #1140
  - new charge conservation tools #1102, #1118, #1132, #1178
  - improve heating tool to support unfinished and single simulations #729
  - support for python3 #1134
  - improve graphics of numerical heating tool #742

  - speed up sliceFieldReader.py #1399
- ionization models:
  - add possibility for starting simulation with neutral atoms #768
  - generalize BSI: rename BSI to BSIHydrogenLike, add BSIStarkShifted and BSIEffectiveZ #1423
  - add ADK (Ammosov-Delone-Krainov) for lin. pol. and circ. pol cases #922 #1490 #1541 #1542
  - add Keldysh #1543
  - make use of faster RNG for Monte-Carlo with ionization #1542 #1543
- support radiation + ionization in LWFA example #868
- PMacc:
  - running with synchronized (blocking) kernels now adds more useful output #725
  - add RNGProvider for persistent PRNG states #1236, #1493
  - add `MRG32k3a` RNG generator #1487
  - move readCheckpointMasterFile to PMacc #1498
  - unify cuda error printing #1484
  - add particle ID provider #1409 #1373
  - split off HostDeviceBuffer from GridBuffer #1370
  - add a policy to GetKeyFromAlias #1252
  - Add border mapping #1133, #1169 #1224
  - make cuSTL gather accept CartBuffers and handle pitches #1196
  - add reference accessors to complex type #1198
  - add more rounding functions #1099
  - add conversion operator from `uint3` to `Dataspace` #1145
  - add more specializations to `GetMPI_StructAsArray` #1088
  - implement cartBuffer conversion for HostBuffer #1092
  - add a policy for async communication #1079
  - add policies for handling particles in guard cells #1077
  - support more types in atomicAddInc and warpBroadcast #1078
  - calculate better seeds #1040 #1046
  - move MallocMCBuffer to PMacc #1034
  - move TypeToPointerPair to PMacc #1033
  - add 1D, 2D and 3D linear interpolation cursor #1217 #1448
  - add method 'getPluginFromType()' to `PluginConnector` #1393
  - math:
    - add `abs`, `asin`, `acos`, `atan`, `log10`, `fmod`, `modf`, `floor` to algorithms::math #837 #1218 #1334 #1362 #1363 #1374 #1473
    - `precisionCast<>` for `PMacc::math::Vector<>` #746
    - support for `boost::mpl::integral_c<>` in `math::CT::Vector<>` #802
    - add complex support #664
  - add `cuSTL/MapTo1DNavigator` #940

  - add 2D support for cuSTL::algorithm::mpi::Gather #844
  - names for exchanges #1511
  - rename EnvMemoryInfo to MemoryInfo #1301
  - mallocMC (*Memory Allocator for Many Core Architectures*) #640 #747 #903 #977 #1171 #1148
    * remove `HeapDataBox`, `RingDataBox`, `HeapBuffer`, `RingBuffer` #640
    * out of heap memory detection #756
    * support to read mallocMC heap on host side #905
  - add multi species support for plugins #794
  - add traits:
    * `GetDataBoxType` #728
    * `FilterByFlag` #1219
    * `GetUniqueTypeId` #957 #962
    * `GetDefaultConstructibleType` #1045
    * `GetInitializedInstance` #1447
    * `ResolveAliasFromSpecies` #1451
    * `GetStringProperties` #1507
  - add pointer class for particles `FramePointer` #1055
  - independent sizes on device for `GridBuffer<>::addExchange`
  - `Communicator`: query periodic directions #1510
  - add host side support for kernel index mapper #902
  - optimize size of particle frame for border frames #949
  - add pre-processor macro for struct generation #972
  - add warp collective atomic function #1013
  - speedup particle operations with collective atomics #1014
  - add support to `deselect` unknown attributes in a particle #1524
  - add `boost.test` #1245
    * test for `HostBufferIntern` #1258
    * test for `setValue()` #1268
- add resource monitor #1456
- add MSVC compatibility #816 #821 #931
- `const` box'es return `const pointer` #945
- refactor host/device identifier #946

Bug Fixes:

- laser implementations:
  - make math calls more robust & portable #1160
  - amplitude of Gaussian beam in 2D3V simulations #1052 #1090
  - avoid non zero E-field integral in plane wave #851
  - fix length setup of plane wave laser #881
  - few-cycle wavepacket #875

  - fix documentaion of `a_0` conversation #1043
- FieldTmp Lamor power calculation #1287
- field solver:
  - stricter condition checks #880
  - 2D3V `NoSolver` did not compile #1073
  - more experimental methods for DS #894
  - experimental: possible out of memory access in directional splitting #890
- moving window moved not exactly with c #1273 #1337 #1549
- 2D3V: possible race conditions for very small, non-default super-cells in current deposition (`StrideMapping`) #1405
- experimental: 2D3V zigzag current deposition fix for `v_z != 0` #823
- vaccuum: division by zero in `Quiet` particle start #1527
- remove variable length arrays #932
- gas (density) profiles:
  - gasFreeFormula #988 #899
  - gaussianCloud #807 #1136 #1265
- C++ should catch by const reference #1295
- fix possible underflow on low memory situations #1188
- C++11 compatibility: use `BOOST_STATIC_CONSTEXPR` where possible #1165
- avoid CUDA 6.5 int(bool) cast bug #680
- PMacc detection in CMake #808
- PMacc:
  - EventPool could run out of free events, potential deadlock #1631
  - Particle<>: avoid using CUDA lmem #1579
  - possible deadlock in event system could freeze simulation #1326
  - HostBuffer includes & constructor #1255 #1596
  - const references in Foreach #1593
  - initialize pointers with NULL before cudaMalloc #1180
  - report device properties of correct GPU #1115
  - rename `types.h` to `pmacc_types.hpp` #1367
  - add missing const for getter in GridLayout #1492
  - Cuda event fix to avoid deadlock #1485
  - use Host DataBox in Hostbuffer #1467
  - allow 1D in CommunicatorMPI #1412
  - use better type for params in vector #1223
  - use correct sqrt function for abs(Vector) #1461
  - fix `CMAKE_PREFIX_PATH`s #1391, #1390
  - remove unnecessary floating point ops from reduce #1212
  - set pointers to NULL before calling cudaMalloc #1180

  - do not allocate memory if not gather root #1181
  - load plugins in registered order #1174
  - C++11 compatibility: use `BOOST_STATIC_CONSTEXPR` where possible #1176 #1175
  - fix usage of `boost::result_of` #1151
  - use correct device number #1115
  - fix vector shrink function #1113
  - split EventSystem.hpp into hpp and tpp #1068
  - fix move operators of CartBuffer #1091
  - missing includes in MapTuple #627
  - GoL example: fix offset #1023
  - remove deprecated throw declarations #1000
  - cuSTL:
    * `cudaPitchedPtr.xsize` used wrong #1234
    * gather for supporting static load balancing #1244
    * reduce #936
    * throw exception on cuda error #1235
    * `DeviceBuffer` assign operator #1375, #1308, #1463, #1435, #1401, #1220, #1197
    * Host/DeviceBuffers: Contructors (Pointers) #1094
    * let kernel/runtime/Foreach compute best BlockDim #1309
  - compile with CUDA 7.0 #748
  - device selection with `process exclusive` enabled #757
  - `math::Vector<>` assignment #806
  - `math::Vector<>` copy constructor #872
  - operator[] in `ConstVector` #981
  - empty `AllCombinations<...>` #1230
  - racecondition in `kernelShiftParticles` #1049
  - warning in `FieldManipulator` #1254
  - memory pitch bug in `MultiBox` and `PitchedBox` #1096
  - `math::abs()` for the type `double` #1470
  - invalid kernel call in `kernelSetValue<>` #1407
  - data alignment for kernel parameter #1566
  - `rsqrt` usage on host #967
  - invalid namespace qualifier #968
  - missing namespace prefix #971
- plugins:
  - radiation:
    * enable multi species for radiation plugin #1454
    * compile issues with math in radiation #1552
    * documentation of radiation observer setup #1422

        * gamma filter in radiation plugin #1421
        * improve vector type name encapsuling #998
        * saveguard restart #716
      - CUDA 7.0+ warning in `PhaseSpace` #750
      - racecondition in `ConcatListOfFrames` #1278
      - illegal memory acces in `Visualisation` #1526
      - HDF5 restart: particle offset overflow fixed #721
  - tools:
      - mpiInfo: add missing include #786
      - actually exit when pression no in compilesuite #1411
      - fix incorrect mangling of params #1385
      - remove deprecated throw declarations #1003
      - make tool python3 compatible #1416
      - trace generating tool #1264
      - png2gas memory leak fixed #1222
      - tbg:
        * quoting interpretation #801
        * variable assignments stay in `.start` files #695 #1609
        * multiple variable use in one line possible #699 #1610
        * failing assignments at template evaluation time keep vars undefined #1611
      - heating tool supports multi species #729
      - fix numerical heating tool normalization #825
      - fix logic behind fill color of numerical heating tool #779
  - libSplash minimum version check #1284

Misc:

  - 2D3V simulations are now honoring the cell "depth" in z to make density interpretations easier #1569
  - update documentation for dependencies and installation #1556, 1557, #1559, #1127
  - refactor usage of several math functions #1462, #1468
  - FieldJ interface clear() replaced with an explicit assign(x) #1335
  - templates for known systems updated:
      - renaming directories into "cluster-insitutition"
      - tbg copies cmakeFlags now #1101
      - tbg aborts if mkdir fails #797
      - `*tpl` & `*.profile.example` files updated
      - system updates: #937 #1266 #1297 #1329 #1364 #1426 #1512 #1443 #1493
        * Lawrencium (LBNL)
        * Titan/Rhea (ORNL)
        * Piz Daint (CSCS)
        * Taurus (TUD) #1081 #1130 #1114 #1116 #1111 #1137

- replace deprecated CUDA calls #758
- remove support for CUDA devices with `sm_10`, `sm_11`, `sm_12` and `sm_13` #813
- remove unused/unsupported/broken plugins #773 843
  - IntensityPlugin, LiveViewPlugin(2D), SumCurrents, divJ #843
- refactor `value_identifier` #964
- remove native type `double` and `float` #985 #990
- remove `__startAtomicTransaction()` #1233
- remove `__syncthreads()` after shared memory allocation #1082
- refactor `ParticleBox` interface #1243
- rotating root in `GatherSlice` (reduce load of master node) #992
- reduce `GatherSlice` memory footprint #1282
- remove `None` type of ionize, pusher #1238 #1227
- remove math function implementations from `Vector.hpp`
- remove unused defines #921
- remove deprecated thow declaration #918
- remove invalid `typename` #917 #933
- rename particle algorithms from `...clone...` to `...derive...` #1525
- remove math functions from Vector.hpp #1472
- raditation plugin remove `unint` with `uint32_t` #1007
- GoL example: CMake modernized #1138
- INSTALL.md
  - moved from `/doc/` to `/`
  - now in root of the repo #1521
  - add environment variable `$PICHOME` #1162
  - more portable #1164
  - arch linux instructions #1065
- refactor ionization towards independence from `Particle` class #874
- update submit templates for hypnos #860 #861 #862
- doxygen config and code modernized #1371 #1388
- cleanup of stdlib includes #1342 #1346 #1347 #1348 #1368 #1389
- boost 1.60.0 only builds in C++11 mode #1315 #1324 #1325
- update minimal CMake version to 3.1.0 #1289
- simplify HostMemAssigner #1320
- add asserts to cuSTL containers #1248
- rename TwistVectorAxes -> TwistComponents (cuSTL) #893
- add more robust namespace qualifiers #839 #969 #847 #974
- cleanup code #885 #814 #815 #915 #920 #1027 #1011 #1009
- correct spelling #934 #938 #941
- add compile test for ALL pushers #1205

- tools:
  - adjust executable rights and shebang #1110 #1107 #1104 #1085 #1143
  - live visualization client added #681 #835 #1408
- CMake
  - modernized #1139
  - only allow out-of-source builds #1119
  - cleanup score-p section #1413
  - add `OpenMP` support #904
- shipped third party updates:
  - restructured #717
  - `cuda_memtest` #770 #1159
  - CMake modules #1087 #1310 #1533
- removed several `-Wshadow` warnings #1039 #1061 #1070 #1071

1.5.16 0.1.0

Date: 2015-05-21

This is version `0.1.0` of PIConGPU, a *pre-beta* version.

Initial field ionization support was added, including the first model for BSI. The code-base was substantially hardened, fixing several minor and major issues. Especially, several restart related issues, an issue with 2D3V zigzack current calculation and a memory issue with Jetson TK1 boards were fixed. A work-around for a critical CUDA 6.5 compiler bug was applied to all affected parts of the code.

Changes to "Open Beta RC6"

.param file changes: See full syntax for each file at https://github.com/ComputationalRadiationPhysics/picongpu/tree/0.1.0/src/pico

- `componentsConfig.param` & `gasConfig.param` fix typo `gasHomogeneous` #577
- `physicalConstants.param`: new variable `GAMMA_THRESH` #669
- `speciesAttributes.param`: new identifier `boundElectrons` and new aliases `ionizer`, `atomicNumbers`
- `ionizationEnergies.param`, `ionizerConfig.param`: added

.unitless file changes: See full syntax for each file at https://github.com/ComputationalRadiationPhysics/picongpu/tree/0.1.0/src/pico

- `gasConfig.unitless`: typo in `gasHomogeneous` #577
- `speciesAttributes.unitless`: new unit for `boundElectrons` identifier
- `speciesDefinition.unitless`: new traits `GetCharge`, `GetMass`, `GetChargeState` and added `ionizers`
- `ionizerConfig.unitless`: added

New Features:

- initial support for field ionization:
  - basic framework and BSI #595
  - attribute (constant flag) for proton and neutron number #687 #731
  - attribute `boundElectrons` #706

- tools:
  - python scripts:
    - new reader for `SliceFieldPrinter` plugin #578
    - new analyzer tool for numerical heating #672 #692
  - `cuda_memtest`:
    - 32bit host system support (Jetson TK1) #583
    - works without `nvidia-smi`, `grep` or `gawk` - optional with NVML for GPU serial number detection (Jetson TK1) #626
  - `splash2txt`:
    - removed build option `S2T_RELEASE` and uses `CMAKE_BUILD_TYPE` #591
  - `tbg`:
    - allows for defaults for `-s`, `-t`, `-c` via env vars #613 #622
  - 3D live visualization: `server` tool that collects `clients` and simulations was published #641
- new/updated particle traits and attributes:
  - `getCharge`, `getMass` #596
  - attributes are now automatically initialized to their generic defaults #607 #615
- PMacc:
  - machine-dependent `UInt` vector class is now split in explicit `UInt32` and `UInt64` classes #665
  - nvidia random number generators (RNG) refactored #711
- plugins:
  - background fields do now affect plugins/outputs #600
  - `Radiation` uses/requires HDF5 output #419 #610 #628 #646 #716
  - `SliceFieldPrinter` supports `FieldJ`, output in one file, updated command-line syntax #548
  - `CountParticles`, `EnergyFields`, `EnergyParticles` support restarts without overwriting their previous output #636 #703

Bug Fixes:

- CUDA 6.5: `int(bool)` casts were broken (affects plugins `BinEnergyParticles`, `PhaseSpace` and might had an effect on methods of the basic PIC cycle) #570 #651 #656 #657 #678 #680
- the ZigZag current solver was broken for 2D3V if non-zero momentum-components in z direction were used (e.g. warm plasmas or purely transversal KHI) #823
- host-device-shared memory (SoC) support was broken (Jetson TK1) #633
- boost 1.56.0+ support via `Resolve<T>` trait #588 #593 #594
- potential race condition in field update and pusher #604
- using `--gridDist` could cause a segfault when adding additional arguments, e.g., in 2D3V setups #638
- `MessageHeader` (used in `png` and 2D live visualization) leaked memory #683
- restarts with HDF5:
  - static load-balancing via `--gridDist` in y-direction was broken #639
  - parallel setups with particle-empty GPUs hung with HDF5 #609 #611 #642
  - 2D3V field reads were broken (each field's z-component was not initialized with the checkpointed values again, e.g., `B_z`) #688 #689
  - loading more than 4 billion global particles was potentially broken #721

- plugins:
  - `Visualization` (png & 2D live sim) memory bug in double precision runs #621
  - `ADIOS`
    - storing more than 4 billion particles was broken #666
    - default of `adios.aggregators` was broken (now = MPI_Size) #662
    - parallel setups with particle-empty GPUs did hang #661
  - `HDF5`/`ADIOS` output of grid-mapped particle energy for non-relativistic particles was zero #669
- PMacc:
  - CMake: path detection could fail #796 #808
  - `DeviceBuffer<*,DIM3>::getPointer()` was broken (does not affect PIConGPU) #647
  - empty super-cell memory foot print reduced #648
  - `float2int` return type should be int #623
  - CUDA 7:
    - cuSTL prefixed templates with _ are not allowed; usage of static dim member #630
    - explicit call to `template`-ed `operator()` to avoid waring #750
    - `EnvironmentController` caused a warning about `extendend friend syntax` #644
  - multi-GPU nodes might fail to start up when not using `default` compute mode with CUDA 7 drivers #643

Misc:

- HDF5 support requires libSplash 1.2.4+ #642 #715
- various code clean-up for MSVC #563 #564 #566 #624 #625
- plugins:
  - removed `LineSliceFields` #590
  - `png` plugin write speedup 2.3x by increasing file size about 12% #698
- updated contribution guidelines, install, cfg examples #601 #598 #617 #620 #673 #700 #714
- updated module examples and cfg files for:
  - lawrencium (LBL) #612
  - titan (ORNL) #618
  - hypnos (HZDR) #670
- an `Empty` example was added, which defaults to the setup given by all `.param` files in default mode (a standard PIC cycle without lasers nor particles), see `src/picongpu/include/simulation_defines/` #634
- some source files had wrong file permissions #668

1.5.17 Open Beta RC6

Date: 2014-11-25

This is the 6th release candidate, a *pre-beta* version.

Initial "multiple species" support was added for flexible particles, but is yet still limited to two species. The checkpoint system was refactored and unified, also incooperating extreme high file I/O bandwidth with ADIOS 1.7+ support. The JetsonTK1 development kit (32bit ARM host side) is now experimentally supported by

PMacc/PIConGPU. The *ZigZag* current deposition scheme was implemented providing 40% to 50% speedup over our optimized Esirkepov implementation.

Changes to "Open Beta RC5"

.param file changes:

- Restructured file output control (HDF5/ADIOS), new `fileOutput.param` #495
- `componentsConfig.param`: particle pushers and current solvers moved to new files:
  - `species.param`: general definitions to change all species at once (pusher, current solver)
  - `pusherConfig.param`: special tweaks for individual particle pushers, forward declarations restructured
  - `particleConfig.param`: shapes moved to `species.param`, still defines initial momentum/temperature
  - `speciesAttributes.param`: defines *unique* attributes that can be used across all particle species
  - `speciesDefinition.param`: finally, assign common attributes from `speciesAttributes.param` and methods from `species.param` to define individual species, also defines a general compile time "list" of all available species
- `currentConfig.param`: removed (contained only forward declarations)
- `particleDefinition.param`: removed, now in `speciesAttributes.param`
- `laserConfig.param`: new polarization/focus sections for plane wave and wave-packet: `git diff --ignore-space-change beta-rc5..beta-rc6 src/picongpu/include/simulation_defines/param/laserConfig.param`
- `memory.param`: remove `TILE_` globals and define general `SuperCellSize` and `MappingDesc` instead #435

.unitless file changes:

- `fileOutput.unitless`: restructured and moved to `fileOutput.param`
- `checkpoint.unitless`: removed some includes
- `currentConfig.unitless`: removed
- `gasConfig.unitless`: calculate 3D gas density (per volume) and 2D surface charge density (per area) #445
- `gridConfig.unitless`: include changed
- `laserConfig.unitless`: added ellipsoid for wave packet
- `physicalConstatns.unitless`: `GAS_DENSITY_NORMED` fixed for 2D #445
- `pusherConfig.unitless`: restructured, according to `pusherConfig.param`
- `memory.unitless`: removed #435
- `particleDefinition.unitless`: removed
- `speciesAttributes.unitless`: added, contains traits to access species attributes (e.g., position)
- `speciesDefinition.unitless`: added, contains traits to access quasi-fixed attributes (e.g., charge/mass)

New Features:

- ZigZag current deposition scheme #436 #476
- initial multi/generic particle species support #457 #474 #516
- plugins

  - BinEnergy supports clean restarts without loosing old files #540
  - phase space now works in 2D3V, with arbitrary super cells and with multiple species #463 #470 #480
  - radiation: 2D support #527 #530
- tools
  - splash2txt now supports ADIOS files #531 #545
- plane wave & wave packet lasers support user-defined polarization #534 #535
- wave packet lasers can be ellipses #434 #446
- central restart file to store available checkpoints #455
- PMacc
  - added `math::erf` #525
  - experimental 32bit host-side support (JetsonTK1 dev kits) #571
  - `CT::Vector` refactored and new methods added #473
  - cuSTL: better 2D container support #461

Bug Fixes:

- esirkepov + CIC current deposition could cause a deadlock in some situations #475
- initialization for `kernelSetDrift` was broken (traversal of frame lists, CUDA 5.5+) #538 #539
- the particleToField deposition (e.g. in FieldTmp solvers for analysis) forgot a small fraction of the particle #559
- PMacc
  - no `static` keyword for non-storage class functions/members (CUDA 6.5+) #483 #484
  - fix a game-of-life compile error #550
  - ParticleBox `setAsLastFrame`/`setAsFirstFrame` race condition (PIConGPU was not affected) #514
- tools
  - tbg caused errors on empty variables, tabs, ampersands, comments #485 #488 #528 #529
- dt/CFL ratio in stdout corrected #512
- 2D live view: fix out-of-mem access #439 #452

Misc:

- updated module examples and cfg files for:
  - hypnos (HZDR) #573 #575
  - taurus (ZIH/TUDD) #558
  - titan (ORNL) #489 #490 #492
- Esirkepov register usage (stack frames) reduced #533
- plugins
  - EnergyFields output refactored and clarified #447 #502
  - warnings fixed #479
  - ADIOS
    - upgraded to 1.7+ support #450 #494
    - meta attributes synchronized with HDF5 output #499
- tools

  - splash2txt updates
    * requires libSplash 1.2.3+ #565
    * handle exceptions more transparently #556
    * fix listing of data sets #549 #555
    * fix warnings #553
  - BinEnergyPlot: refactored #542
  - memtest: warnings fixed #521
  - pic2xdmf: refactor XDMF output format #503 #504 #505 #506 #507 #508 #509
  - paraview config updated for hypnos #493
- compile suite
  - reduce verbosity #467
  - remove virtual machine and add access-control list #456 #465
- upgraded to ADIOS 1.7+ support #450 #494
- boost 1.55.0 / nvcc <6.5 work around only applied for affected versions #560
- `boost::mkdir` is now used where necessary to increase portability #460
- PMacc
  - `ForEach` refactored #427
  - plugins: `notify()` is now called *before* `checkpoint()` and a getter method was added to retrieve the last call's time step #541
  - `DomainInfo` and `SubGrid` refactored and redefined #416 #537
  - event system overhead reduced by 3-5% #536
  - warnings fixed #487 #515
  - cudaSetDeviceFlags: uses `cudaDeviceScheduleSpin` now #481 #482
  - `__delete` makro used more consequently #443
  - static asserts refactored and messages added #437
- coding style / white space cleanups #520 #522 #519
- git / GitHub / documentation
  - pyc (compiled python files) are now ignored #526
  - pull requests: description is mandatory #524
- mallocMC cmake `find_package` module added #468

1.5.18 Open Beta RC5

Date: 2014-06-04

This is the 5th release candidate, a *pre-beta* version.

We rebuild our complete plugin and restart scheme, most of these changes are not backwards compatible and you will have to upgrade to libSplash 1.2+ for HDF5 output (this just means: you can not restart from a beta-rc4 checkpoint with this release).

HDF5 output with libSplash does not contain *ghost*/*guard* data any more. These information are just necessary for checkpoints (which are now separated from the regular output).

Changes to "Open Beta RC4"

.param file changes:

- Added selection of optional window functions in `radiationConfig.param` #286
- Added more window functions in `radiationConfig.param` #320
- removed double `#define __COHERENTINCOHERENTWEIGHTING__ 1` in some examples `radiationConfig.param` #323
- new file: `seed.param` allows to vary the starting conditions of "identical" runs #353
- Updated a huge amount of `.param` files to remove outdated comments #384
- Update `gasConfig.param`/`gasConfig.unitless` and doc string in `componentsConfig.param` with new gasFromHdf5 profile #280

.unitless file changes:

- update `fileOutput.unitless` and add new file `checkpoints.unitless` #387
- update `fieldSolver.unitless` #314
- Update `radiationConfig.unitless`: adjust to new supercell size naming #394
- Corrected CFL criteria (to be less conservative) in `gridConfig.unitless` #371

New Features:

- Radiation plugin: add optional window functions to reduce ringing effects caused by sharp boundaries #286 #323 #320
- load gas profiles from png #280
- restart mechanism rebuild #326 #375 #358 #387 #376 #417
- new unified naming scheme for domain and window sizes/offsets #128 #334 #396 #403 #413 #421
- base seed for binary idential simulations now exposed in seed.param #351 #353
- particle kernels without "early returns" #359 #360
- lowered memory foot print during shiftParticles #367
- ShiftCoordinateSystem refactored #414
- tools:
  - tbg warns about broken line continuations in tpl files #259
  - new CMake modules for: ADIOS, libSplash, PNGwriter #271 #304 #307 #308 #406
  - pic2xdmf
    - supports information tags #290 #294
    - one xdmf for grids and one for particles #318 #345
  - Vampir and Score-P support updated/added #293 #291 #399 #422
  - ParaView remote server description for Hypnos (HZDR) added #355 #397
- plugins
  - former name: "modules" #283
  - completely refactored #287 #336 #342 #344
  - restart capabilites added (partially) #315 #326 #425
  - new 2D phase space analysis added (for 3D sims and one species at a time) #347 #364 #391 #407
  - libSplash 1.2+ upgrade (incompatible output to previous versions) #388 #402
- PMacc

  - new Environment class provides all singletons #254 #276 #404 #405
  - new particle traits, methods and flags #279 #306 #311 #314 #312
  - cuSTL ForEach on 1-3D data sets #335
  - cuSTL twistVectorAxes refactored #370
  - NumberOfExchanges replaced numberOfNeighbors implementation #362
  - new math functions: tan, float2int_rd (host) #374 #410
  - CT::Vector now supports ::shrink #392

Bug fixes:

- CUDA 5.5 and 6.0 support was broken #401
- command line argument parser messages were broken #281 #270 #309
- avoid deadlock in computeCurrent, remove early returns #359
- particles that move in the absorbing GUARD are now cleaned up #363
- CFL criteria fixed (the old one was too conservative) #165 #371 #379
- non-GPU-aware (old-stable) MPI versions could malform host-side pinned/page-locked buffers for subsequent cudaMalloc/cudaFree calls (core routines not affected) #438
- ADIOS
  - particle output was broken #296
  - CMake build was broken #260 #268
- libSplash
  - output performance drastically improved #297
- PMacc
  - GameOfLife example was broken #295
  - log compile broken for high log level #372
  - global reduce did not work for references/const #448
  - cuSTL assign was broken for big data sets #431
  - cuSTL reduce minor memory leak fixed #433
- compile suite updated and messages escaped #301 #385
- plugins
  - BinEnergyParticles header corrected #317 #319
  - PNG undefined buffer values fixed #339
  - PNG in 2D did not ignore invalid slides #432
- examples
  - Kelvin-Helmholtz example box size corrected #352
  - Bunch/SingleParticleRadiationWithLaser observation angle fixed #424

Misc:

- more generic 2 vs 3D algorithms #255
- experimental PGI support removed #257
- gcc 4.3 support dropped #264
- various gcc warnings fixed #266 #284

- CMake 3.8.12-2 warnings fixed #366
- picongpu.profile example added for
  - Titan (ORNL) #263
  - Hypnos (HZDR) #415
- documentation updated #275 #337 #338 #357 #409
- wiki started: plugins, developer hints, simulation control, examples #288 #321 #328
- particle interfaces clened up #278
- ParticleToGrid kernels refactored #329
- slide log is now part of the SIMULATION_STATE level #354
- additional NGP current implementation removed #429
- PMacc
  - GameOfLife example documented #305
  - compile time vector refactored #349
  - shortened compile time template error messages #277
  - cuSTL inline documentation added #365
  - compile time operators and ForEach refactored #380
  - TVec removed in preference of CT::Vector #394
- new developers added #331 #373
- Attribution text updated and BibTex added #428

1.5.19 Open Beta RC4

Date: 2014-03-07

This is the 4th release candidate, a *pre-beta* version.

Changes to "Open Beta RC3"

.param file changes:

- Removed unnesseary includes #234 from: `observer.hpp`, `physicalConstants.param`, `visColorScales.param`, `visualization.param`, `particleConfig.param`, `gasConfig.param`, `fieldBackground.param`, `particleDefinition.param` see the lines that should be removed in #234
- Renamed `observer.hpp` -> `radiationObserver.param` #237 #241 Changed variable name `N_theta` to `N_observer` https://github.com/ComputationalRadiationPhysics/picongpu/commit/9e487ec30ade10ece44fc19
9
- Added background FieldJ (current) capability #245 Add the following lines to your `fieldBackground.param`: https://github.com/ComputationalRadiationPhysics/picongpu/commit/7b22f37c6a58250d6623cfbc821c4f996145aad
1

New Features:

- 2D support for basic PIC cycle #212
- hdf5 output xdmf meta description added: ParaView/VisIt support #219
- background current (FieldJ) can be added now #245

Bug fixes:

- beta-rc3 was broken for some clusters due to an init bug #239
- examples/WeibelTransverse 4 GPU example was broken #221
- smooth script was broken for 1D fields #223
- configure non-existing path did not throw an error #229
- compile time vector "max" was broken #224
- cuda_memtest did throw false negatives on hypnos #231 #236
- plugin "png" did not compile for missing freetype #248

Misc:

- documentation updates
  - radiation post processing scripts #222
  - more meta data in hdf5 output #216
  - tbg help extended and warnings to errors #226
  - doc/PARTICIPATE.md is now GitHub's CONTRIBUTING.md #247 #252
  - slurm interactive queue one-liner added #250
  - developers updated #251
- clean up / refactoring
  - cell_size -> cellSize #227
  - typeCast -> precisionCast #228
  - param file includes (see above for details) #234
  - DataConnector interface redesign #218 #232
  - Esirkepov implementation "paper-like" #238

1.5.20 Open Beta RC3

Date: 2014-02-14

This is the third release candidate, a *pre-beta* version.

Changes to "Open Beta RC2"

.param and .cfg file changes:

- `componentsConfig.param`:
  - remove simDim defines #134 #137 (example how to update your existing `componentsConfig.param`, see https://github.com/ComputationalRadiationPhysics/picongpu/commit/af1f20790ad2aa15e6fc2c9a51d8c870
- `dimension.param`: new file with simDim setting #134
  - only add this file to your example/test/config if you want to change it from the default value (3D)
- `fieldConfig.param`: renamed to `fieldSolver.param` #131
- `fieldBackground.param`: new file to add external background fields #131
- cfg files cleaned up #153 #193

New Features:

- background fields for E and B #131
- write parallel hdf5 with libSplash 1.1 #141 #151 #156 #191 #196

- new plugins
  - ADIOS output support #179 #196
  - makroParticleCounter/PerSuperCell #163
- cuda_memtest can check mapped memory now #173
- EnergyDensity works for 2-3D now #175
- new type floatD_X shall be used for position types (2-3D) #184
- PMacc
  - new functors for multiplications and substractions #135
  - opened more interfaces to old functors #197
  - MappedMemoryBuffer added #169 #182
  - unary transformations can be performed on DataBox'es now, allowing for non-commutative operations in reduces #204

Bug fixes:

- PMacc
  - GridBuffer could deadlock if called uninitialized #149
  - TaskSetValue was broken for all arrays with x-size != n*256 #174
  - CUDA 6.0 runs crashed during cudaSetDeviceFlags #200
  - extern shared mem could not be used with templated types #199
- tbg
  - clearify error message if the tpl file does not exist #130
- HDF5Writer did not write ions any more #188
- return type of failing Slurm runs fixed #198 #205
- particles in-cell position fixed with cleaner algorithm #209

Misc:

- documentation improved for
  - cuSTL #116
  - gasConfig.param describe slopes better (no syntax changes) #126
  - agreed on coding guide lines #155 #161 #140
  - example documentation started #160 #162 #176
  - taurus (slurm based HPC cluster) updates #206
- IDE: ignore Code::Blocks files #125
- Esirkepov performance improvement by 30% #139
- MySimulation asserts refactored for nD #187
- Fields.def with field forward declarations added, refactored to provide common ValueType #178
- icc warnings in cuda_memcheck fixed #210
- PMacc
  - refactored math::vector to play with DataSpace #138 #147
  - addLicense script updated #167
  - MPI_CHECK writes to stderr now #168

  - TVec from/to CT::Int conversion #185
  - PositionFilter works for 2-3D now #189 #207
  - DeviceBuffer cudaPitchedPtr handling clean up #186
  - DataBoxDim1Access refactored #202

1.5.21 Open Beta RC2

Date: 2013-11-27

This is the second release candidate, a *pre-beta* version.

Changes to "Open Beta RC1"

.param file changes:

- `gasConfig.param`:
  - add gasFreeFormula #96 (example how to update your existing `gasConfig.param`, see https://github.com/ComputationalRadiationPhysics/picongpu/pull/96/files#diff-1)
  - add inner radius to gasSphereFlanks #66 (example how to update your existing `gasConfig.param`, see https://github.com/ComputationalRadiationPhysics/picongpu/pull/66/files#diff-0)

New Features:

- A change log was introduced for master releases #93
- new gas profile "gasFreeFormula" for user defined profiles #96
- CMake (config) #79
  - checks for minimal required versions of dependent libraries #92
  - checks for libSplash version #85
  - update to v2.8.5+ #52
  - implicit plugin selection: enabled if found #52
  - throw more warnings #37
  - experimental support for icc 12.1 and PGI 13.6 #37
- PMacc
  - full rewrite of the way we build particle frames # 86
  - cuSTL: ForEach works on host 1D and 2D data now #44
  - math::pow added #54
  - compile time ForEach added #50
- libSplash
  - dependency upgraded to beta (v1.0) release #80
  - type traits for types PIConGPU - libSplash #69
  - splash2txt update to beta interfaces #83
- new particle to grid routines calculating the Larmor energy #68
- dumping multiple FieldTmp to hdf5 now possible #50
- new config for SLURM batch system (taurus) #39

Bug fixes:

- PMacc
  - cuSTL
    - assign was broken for deviceBuffers #103
    - lambda expressions were broken #42 #46 #100
    - icc support was broken #100 #101
    - views were broken #62
  - InheritGenerator and deselect: icc fix #101
  - VampirTrace (CUPTI) support: cudaDeviceReset added #90
  - GameOfLife example fixed #53 #55
  - warnings in __cudaKernel fixed #51
- picongpu
  - removed all non-ascii chars from job scripts #95 #98
  - CMake
    - keep ptx code was broken #82
    - PGI: string compare broken #75
    - MPI: some libs require to load the C++ dependencies, too #64
    - removed deprecated variables #52
    - Threads: find package was missing #34
  - various libSplash bugs #78 #80 #84
  - current calculation speedup was broken #72
  - Cell2Particle functor missed to provide static methods #49
- tools
  - compile: script uses -q now implicit for parallel (-j N) tests
  - plotDensity: update to new binary format #47
- libraries
  - boost 1.55 work around, see trac #9392 (nvcc #391854)

Misc:

- new reference: SC13 paper, Gordon Bell Finals #106
- new flavoured logo for alpha
- Compile Suite: GitHub integration #33 #35
- dropped CUDA sm_13 support (now sm_20+ is required) #42

1.5.22 Open Beta RC1

Date: 2013-09-05 07:47:03 -0700

This is the first release candidate, a *pre-beta* version. We tagged this state since we started to support `sm_20+` only.

Changes to "Open Alpha"

n/a

1.5.23 Open Alpha

Date: 2013-08-14 02:25:36 -0700

That's our our open alpha release. The alpha release is **developer** and **power user** release only! **Users** should wait for our beta release!

CHAPTER

TWO

USAGE

2.1 Reference

Section author: Axel Huebl

PIConGPU is an almost decade-long scientific project with many people contributing to it. In order to credit the work of others, we expect you to cite our latest paper describing PIConGPU when publishing and/or presenting scientific results.

In addition to that and out of good scientific practice, you should document the version of PIConGPU that was used and any modifications you applied. A list of releases alongside a DOI to reference it can be found here:

https://github.com/ComputationalRadiationPhysics/picongpu/releases

2.1.1 Citation

BibTeX code:

```
@inproceedings{PIConGPU2013,
 author = {Bussmann, M. and Burau, H. and Cowan, T. E. and Debus, A. and Huebl, A.␣
↪and Juckeland, G. and Kluge, T. and Nagel, W. E. and Pausch, R. and Schmitt, F.␣
↪and Schramm, U. and Schuchart, J. and Widera, R.},
 title = {Radiative Signatures of the Relativistic Kelvin-Helmholtz Instability},
 booktitle = {Proceedings of the International Conference on High Performance␣
↪Computing, Networking, Storage and Analysis},
 series = {SC '13},
 year = {2013},
 isbn = {978-1-4503-2378-9},
 location = {Denver, Colorado},
 pages = {5:1--5:12},
 articleno = {5},
 numpages = {12},
 url = {http://doi.acm.org/10.1145/2503210.2504564},
 doi = {10.1145/2503210.2504564},
 acmid = {2504564},
 publisher = {ACM},
 address = {New York, NY, USA},
}
```

2.1.2 Acknowledgements

In many cases you receive support and code base maintainance from us or the PIConGPU community without directly justifying a full co-authorship. Additional to the citation, please consider adding an acknowledgement of the following form to reflect that:

> We acknowledge all contributors to the open-source code PIConGPU for enabling our simulations.

or:

> We acknowledge [list of specific persons that helped you] and all further contributors to the open-source code PIConGPU for enabling our simulations.

2.1.3 Community Map

PIConGPU comes without a registration-wall, with open and re-distributable licenses and without any strings attached. We therefore *rely on you* to show our community, diversity and usefulness, e.g. to funding agencies.

> Please consider adding yourself to our community map!

Thank you and enjoy PIConGPU and our community!

2.1.4 Publications

The following publications are sorted by topics. Papers covering multiple topics will be listed multiple times. In the end, a list of all publications in chronological order is given with more details. If you want to add your publication to the list as well please feel free to contact us or open a pull request directly.

Application of PIConGPU in various physics scenarios

In the following, a list of publications describing using PIConGPU is given in various cases.

Laser plasma electron acceleration

- Laser wakefield acceleration (LWFA) with self-truncated ionization-injection (STII) [Couperus2017]
- PhD thesis on experimental aspects of LWFA with STII [Couperus2018],
- PhD thesis on theoretical ascpects of self-focusing during LWFA with STII [Pausch2019]
- Hybrid laser-driven/beam-driven plasms acceleration [Kurz2021]

Laser plasma ion acceleration

- Proton acceleration from cryogenic hydrogen jets [Obst2017]
- Mass-Limited, Near-Critical, micron-scale, spherical targets [Hilz2018]
- PhD thesis on theoretical aspects of mass-limited, near-critical, micron-scale, spherical targets [Huebl2019]
- All-optical stuctering of laser-accelerated protons [Obst-Huebl2018]
- PhD thesis on laser-driven proton beam structering [Obst-Huebl2019]
- Laser-ion multi-species acceleration [Huebl2020]

Laser plasma light sources and diagnostics

- PhD thesis on radiation from LWFA [Pausch2019]
- Laser-driven x-ray and proton sources [Ostermayr2020]
- Betatron x-ray diagnostic for beam decoherence [Koehler2019], [Koehler2021]

Astrophysics

- Simulating the Kelvin Helmholtz instability (KHI) [Bussmann2013]
- Visualizing the KHI [Huebl2014]
- Theoretical model of the radiation evolution during the KHI [Pausch2017]
- PhD thesis covering the KHI radiation [Pausch2019]

Machine Learning

Methods used in PIConGPU software

In the following, a list of references is given, sorted by topics, that describe PIConGPU as a software. References to publications of implemented methods that were developed by other groups are also given for completeness. These references are marked by an asterisk.

General code references

- First publication on PIConGPU [Burau2010]
- Currently main reference [Bussmann2013]
- Most up-to-date reference [Huebl2019]

Field solvers

- Yee field solver* [Yee1966]
- Lehe fields solver* [Lehe2013]
- High-Order Finite Difference solver* [Ghrist2000]

Particle pushers

- Boris pusher* [Boris1970]
- Vay pusher* [Vay2008]
- Reduces Landau-Lifshitz pusher* [Vranic2016]
- Higuera-Cary pusher [Higuera2017]

Current deposition

- Esirkepov method* [Esirkepov2001]
- Villasenor and Buneman method* [Villasenior1991]

Ionization-physics extensions

- Barrier suppression ionization (BSI)* [ClementiRaimondi1963], [ClementiRaimondi1967], [MulserBauer2010]
- Tunneling ionization - Keldysh* [Keldysh]
- Tunneling ionization - Ammosov-Delone-Krainov (ADK)* [DeloneKrainov1998], [BauerMulser1999]

- Master thesis - model implementation [Garten2015]
- Collisional ionization [FLYCHK2005], [More1985]
- ionization current* [Mulser1998]

Binary_collisions

- fundamental alogorithm* [Perez2012]
- improvements and corrections* [Higginson2020]

QED code extensions

- Various methods applicable in PIC codes* [Gonoskov2015]
- Diploma thesis - model implementation [Burau2016]

Diagnostic methods

- classical radiation: [Pausch2012], [Pausch2014], [Pausch2018], [Pausch2019]
- phase space analysis: [Huebl2014]
- beam emittance: [Rudat2019]
- coherent transistion radiation (CTR): [Carstens2019]

Visualization

- first post-processing implementation: [Zuehl2011], [Ungethuem2012]
- first in-situ visualization: [Schneider2012a], [Schneider2012b]
- Kelvin-Helmholtz instabilty: [Huebl2014]
- in-situ visualization with ISAAC: [Matthes2016], [Matthes2016b]
- in-situ particle rendering: [Meyer2018]

Input/Output

- parallel HDF5, ADIOS1, compression, data reduction and I/O performance model [Huebl2017]

HPC kernels and benchmarks

- proceedings of the SC'13 [Bussmann2013]

Theses

- Diploma thesis: first post-processing rendering [Zuehl2011]
- Diploma thesis: first in-situ rendering [Schneider2012b]
- Diploma thesis: In-situ radiation calculation [Pausch2012]
- Diploma thesis: Algorithms, LWFA injection, Phase Space analysis [Huebl2014]
- Master thesis: Ionization methods [Garten2015]

- Diploma thesis: QED scattering processes [Burau2016]
- Diploma thesis: In-situ live visualization [Matthes2016]
- PhD thesis: LWFA injection using STII (mainly experiment) [Couperus2018]
- Bachelor thesis: In-situ live visualization [Meyer2018]
- Master thesis: Beam emittance and automated parameter scans [Rudat2019]
- PhD thesis: Radiation during LWFA and KHI, radiative corrections [Pausch2019]
- PhD thesis: LWFA betatron radiation (mainly experiment) [Koehler2019]
- PhD thesis: LWFA Coherent transistion radiation diagnostics (CTR) (mainly experiment) [Zarini2019]
- PhD thesis: Laser ion acceleration (mainly experiment) [Obst-Huebl2019]
- PhD thesis: Exascale simulations with PIConGPU, laser ion acceleration [Huebl2019]
- Bachelor thesis: Synthetic coherent transistion radiation [Carstens2019]

List of PIConGPU references in chronological order

List of other references in chronological order

See also:

You need to have an *environment loaded* (`source $HOME/picongpu.profile` when installing from source or `spack load picongpu` when using spack) that provides all *PIConGPU dependencies* to complete this chapter.

Warning: PIConGPU source code is portable and can be compiled on all major operating systems. However, helper tools like `pic-create` and `pic-build` described in this section rely on Linux utilities and thus are not expected to work on other platforms out-of-the-box. Note that building and using PIConGPU on other operating systems is still possible but has to be done manually or with custom tools. This case is not covered in the documentation, but we can assist users with it when needed.

2.2 Basics

Section author: Axel Huebl

2.2.1 Preparation

First, decide where to store input files, a good place might be `$HOME` (`~`) because it is usually backed up. Second, decide where to store your output of simulations which needs to be placed on a high-bandwidth, large-storage file system which we will refer to as `$SCRATCH`.

For a first test you can also use your home directory:

```
export SCRATCH=$HOME
```

We need a few directories to structure our workflow:

```
# PIConGPU input files
mkdir $HOME/picInputs

# PIConGPU simulation output
mkdir $SCRATCH/runs
```

2.2.2 Step-by-Step

1. Create an Input (Parameter) Set

```
# clone the LWFA example to $HOME/picInputs/myLWFA
pic-create $PIC_EXAMPLES/LaserWakefield $HOME/picInputs/myLWFA

# switch to your input directory
cd $HOME/picInputs/myLWFA
```

PIConGPU is controlled via two kinds of textual input sets: compile-time options and runtime options.

Compile-time *.param files* reside in `include/picongpu/param/` and define the physics case and deployed numerics. After creation and whenever options are changed, PIConGPU *requires a re-compile*. Feel free to take a look now, but we will later come back on how to *edit those files*.

Runtime (command line) arguments are set in `etc/picongpu/*.cfg` files. These options do *not* require a re-compile when changed (e.g. simulation size, number of devices, plugins, ...).

2. Compile Simulation

In our input, `.param` files are build directly into the PIConGPU binary for *performance reasons*. A compile is required after changing or initially adding those files.

In this step you can optimize the simulation for the specific hardware you want to run on. By default, we compile for Nvidia GPUs with the CUDA backend, targeting the oldest compatible architecture.

```
pic-build
```

This step will take a few minutes. Time for a coffee or a sword fight!

We explain in the *details section* below how to set further options, e.g. CPU targets or tuning for newer GPU architectures.

3. Run Simulation

While you are still in `$HOME/picInputs/myLWFA`, start your simulation on one CUDA capable GPU:

```
# example run for an interactive simulation on the same machine
tbg -s bash -c etc/picongpu/1.cfg -t etc/picongpu/bash/mpiexec.tpl $SCRATCH/runs/
↪lwfa_001
```

This will create the directory `$SCRATCH/runs/lwfa_001` where all simulation output will be written to. `tbg` will further create a subfolder `input/` in the directory of the run with the same structure as `myLWFA` to archive your input files. Subfolder `simOutput/` has all the simulation results. Particularly, the simulation progress log is in `simOutput/output`.

4. Creating Own Simulation

For creating an own simulation, we recommend starting with the most fitting example and modifying the *compile-time options in .param files* and *run-time options in .cfg files*. Changing contents of `.param` files requires recompilation of the code, modifying `.cfg` files does not. Note that available run-time options generally depend on the environment used for the build, the chosen compute backend, and the contents of `.param` files. To get the list of all available options for the current configuration, after a successful `pic-build` run

```
.build/picongpu --help
```

2.2.3 Details on the Commands Above

tbg

The `tbg` tool is explained in detail *in its own section*. Its primary purpose is to abstract the options in runtime `.cfg` files from the technical details on how to run on various supercomputers.

For example, if you want to run on the HPC System "Hemera" at HZDR, your `tbg` submit command would just change to:

```
# request 1 GPU from the PBS batch system and run on the queue "k20"
tbg -s sbatch -c etc/picongpu/1.cfg -t etc/picongpu/hemera-hzdr/k20.tpl $SCRATCH/
↪runs/lwfa_002

# run again, this time on 16 GPUs
tbg -s sbatch -c etc/picongpu/16.cfg -t etc/picongpu/hemera-hzdr/k20.tpl $SCRATCH/
↪runs/lwfa_003
```

Note that we can use the same `1.cfg` file, your input set is *portable*.

pic-create

This tool is just a short-hand to create a new set of input files. It copies from an already existing set of input files (e.g. our examples or a previous simulation) and adds additional helper files.

See `pic-create --help` for more options during input set creation:

```
pic-create create a new parameter set for simulation input
merge default picongpu parameters and a given example's input

usage: pic-create [OPTION] [src_dir] dest_dir
If no src_dir is set picongpu a default case is cloned
If src_dir is not in the current directory, pic-create will
look for it in $PIC_EXAMPLES

-f | --force         - merge data if destination already exists
-h | --help          - show this help message

Dependencies: rsync
```

A run simulation can also be reused to create derived input sets via `pic-create`:

```
pic-create $SCRATCH/runs/lwfa_001/input $HOME/picInputs/mySecondLWFA
```

pic-build

This tool is actually a short-hand for an *out-of-source build with CMake*.

In detail, it does:

```
# go to an empty build directory
mkdir -p .build
cd .build

# configure with CMake
pic-configure $OPTIONS ..

# compile PIConGPU with the current input set (e.g. myLWFA)
# - "make -j install" runs implicitly "make -j" and then "make install"
# - make install copies resulting binaries to input set
make -j install
```

`pic-build` accepts the same command line flags as *pic-configure*. For example, if you want to build for running on CPUs instead of a GPUs, call:

```
# example for running efficiently on the CPU you are currently compiling on
pic-build -b "omp2b"
```

Its full documentation from `pic-build --help` reads:

```
Build new binaries for a PIConGPU input set

Creates or updates the binaries in an input set. This step needs to
be performed every time a .param file is changed.

This tools creates a temporary build directory, configures and
compiles current input set in it and installs the resulting
binaries.
This is just a short-hand tool for switching to a temporary build
directory and running 'pic-configure ..' and 'make install'
manually.

You must run this command inside an input directory.

usage: pic-build [OPTIONS]

-b | --backend       - set compute backend and optionally the architecture
                       syntax: backend[:architecture]
                       supported backends: cuda, hip, omp2b, serial, tbb, threads
                       (e.g.: "cuda:35;37;52;60" or "omp2b:native" or "omp2b")
                       default: "cuda" if not set via environment variable PIC_
↪BACKEND
                       note: architecture names are compiler dependent
-c | --cmake         - overwrite options for cmake
                       (e.g.: "-DPIC_VERBOSE=21 -DCMAKE_BUILD_TYPE=Debug")
-t <presetNumber>    - configure this preset from cmakeFlags
-f | --force         - clear the cmake file cache and scan for new param files
-h | --help          - show this help message
```

pic-configure

This tool is just a convenient wrapper for a call to CMake. It is executed from an *empty build directory*.

You will likely not use this tool directly. Instead, *pic-build* from above calls `pic-configure` for you, forwarding its arguments.

We *strongly recommend* to set the appropriate target compute backend via `-b` for optimal performance. For Nvidia CUDA GPUs, set the compute capability of your GPU:

```
# example for running efficiently on a K80 GPU with compute capability 3.7
pic-configure -b "cuda:37" $HOME/picInputs/myLWFA
```

For running on a CPU instead of a GPU, set this:

```
# example for running efficiently on the CPU you are currently compiling on
pic-configure -b "omp2b:native" $HOME/picInputs/myLWFA
```

Note: If you are compiling on a cluster, the CPU architecture of the head/login nodes versus the actual compute architecture does likely vary! Compiling a backend for the wrong architecture does in the best case dramatically reduce your performance and in the worst case will not run at all!

During configure, the backend's architecture is forwarded to the compiler's `-mtune` and `-march` flags. For example, if you are compiling with GCC for running on *AMD Opteron 6276 CPUs* set `-b omp2b:bdver1` or

for *Intel Xeon Phi Knight's Landing CPUs* set `-b omp2b:knl`.

See `pic-configure --help` for more options during input set configuration:

```
Configure PIConGPU with CMake

Generates a call to CMake and provides short-hand access to selected
PIConGPU CMake options.
Advanced users can always run 'ccmake .' after this call for further
compilation options.

usage: pic-configure [OPTIONS] <inputDirectory>

-i | --install       - path were picongpu shall be installed
                       (default is <inputDirectory>)
-b | --backend       - set compute backend and optionally the architecture
                       syntax: backend[:architecture]
                       supported backends: cuda, hip, omp2b, serial, tbb, threads
                       (e.g.: "cuda:35;37;52;60" or "omp2b:native" or "omp2b")
                       default: "cuda" if not set via environment variable PIC_
↪BACKEND
                       note: architecture names are compiler dependent
-c | --cmake         - overwrite options for cmake
                       (e.g.: "-DPIC_VERBOSE=21 -DCMAKE_BUILD_TYPE=Debug")
-t <presetNumber>    - configure this preset from cmakeFlags
-f | --force         - clear the cmake file cache and scan for new param files
-h | --help          - show this help message
```

After running configure you can run `ccmake .` to set additional compile options (optimizations, debug levels, hardware version, etc.). This will influence your build done via `make install`.

You can pass further options to configure PIConGPU directly instead of using `ccmake .`, by passing `-c "-DOPTION1=VALUE1 -DOPTION2=VALUE2"`.

2.3 .param Files

Section author: Axel Huebl

Parameter files, `*.param` placed in `include/picongpu/param/` are used to set all **compile-time options** for a PIConGPU simulation. This includes most fundamental options such as numerical solvers, floating precision, memory usage due to attributes and super-cell based algorithms, density profiles, initial conditions etc.

2.3.1 Editing

For convenience, we provide a tool `pic-edit` to edit the compile-time input by its name. For example, if you want to edit the *grid* and time step resolution, *file output* and add a *laser* to the simulation, open the according files via:

```
# first switch to your input directory
cd $HOME/picInputs/myLWFA

pic-edit grid fileOutput laser
```

See `pic-edit --help` for all available files:

```
Edit compile-time options for a PIConGPU input set

Opens .param files in an input set with the default "EDITOR".
```

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```
If a .param file is not yet part of the input set but exists in the
defaults, it will be transparently added to the input set.

You must run this command inside an input directory.

The currently selected editor is: /usr/bin/vim.basic
You can change it via the "EDITOR" environment variable.

usage: pic-edit <input>

Available <input>s:
bremsstrahlung collision components density dimension fieldAbsorber␣
↪fieldBackground fieldSolver fileOutput flylite grid incidentField␣
↪ionizationEnergies ionizer isaac iterationStart laser mallocMC memory particle␣
↪particleCalorimeter particleFilters particleMerger physicalConstants png␣
↪pngColorScales precision pusher radiation radiationObserver random species␣
↪speciesAttributes speciesConstants speciesDefinition speciesInitialization␣
↪starter synchrotronPhotons transitionRadiation unit xrayScattering
```

2.3.2 Rationale

High-performance hardware comes with a lot of restrictions on how to use it, mainly memory, control flow and register limits. In order to create an efficient simulation, PIConGPU compiles to **exactly** the numerical solvers (kernels) and physical attributes (fields, species) for the setup you need to run, which will furthermore be specialized for a specific hardware.

This comes at a small cost: when **even one of those settings is changed, you need to recompile**. Nevertheless, wasting about 5 minutes compiling on a single node is nothing compared to the time you save *at scale*!

All options that are less or non-critical for runtime performance, such as specific ranges observables in *plugins* or how many nodes shall be used, can be set in *run time configuration files (*.cfg)* and do not need a recompile when changed.

2.3.3 Files and Their Usage

If you use our `pic-configure` *script wrappers*, you do not need to set *all* available parameter files since we will add the missing ones with *sane defaults*. Those defaults are:

- a standard, single-precision, well normalized PIC cycle suitable for relativistic plasmas
- no external forces (no laser, no initial density profile, no background fields, etc.)

2.3.4 All Files

When setting up a simulation, it is recommended to adjust `.param` files in the following order:

PIC Core

dimension.param

The spatial dimensionality of the simulation.

Defines

`SIMDIM`
: Possible values: DIM3 for 3D3V and DIM2 for 2D3V.

namespace picongpu

Variables

constexpr uint32_t **simDim** = SIMDIM

grid.param

Definition of cell sizes and time step.

Our cells are defining a regular, cartesian grid. Our explicit FDTD field solvers require an upper bound for the time step value in relation to the cell size for convergence. Make sure to resolve important wavelengths of your simulation, e.g. shortest plasma wavelength, Debye length and central laser wavelength both spatially and temporarily.

Units in reduced dimensions

In 2D3V simulations, the CELL_DEPTH_SI (Z) cell length is still used for normalization of densities, etc..

A 2D3V simulation in a cartesian PIC simulation such as ours only changes the degrees of freedom in motion for (macro) particles and all (field) information in z travels instantaneously, making the 2D3V simulation behave like the interaction of infinite "wire particles" in fields with perfect symmetry in Z.

namespace picongpu

namespace SI

Variables

constexpr float_64 **DELTA_T_SI** = 0.8e-16
Duration of one timestep unit: seconds.

constexpr float_64 **CELL_WIDTH_SI** = 0.1772e-6
equals X unit: meter

constexpr float_64 **CELL_HEIGHT_SI** = 0.4430e-7
equals Y - the laser & moving window propagation direction unit: meter

constexpr float_64 **CELL_DEPTH_SI** = *CELL_WIDTH_SI*
equals Z unit: meter

components.param

Select a user-defined simulation class here, e.g.

with strongly modified initialization and/or PIC loop beyond the parametrization given in other .param files.

namespace simulation_starter
Simulation Starter Selection: This value does usually not need to be changed.

Change only if you want to implement your own `SimulationHelper` (e.g. `Simulation`) class.

- defaultPIConGPU : default PIConGPU configuration

iterationStart.param

Specify a sequence of functors to be called at start of each time iteration.

namespace picongpu

Typedefs

using IterationStartPipeline = bmpl::vector<>
IterationStartPipeline defines the functors called at each iteration start.

The functors will be called in the given order.

The functors must be default-constructible and take the current time iteration as the only parameter. These are the same requirements as for functors in particles::InitPipeline.

fieldSolver.param

Configure the field solver.

Select the numerical Maxwell solver (e.g. Yee's method).

Attention Currently, the laser initialization in PIConGPU is implemented to work with the standard Yee solver. Using a solver of higher order will result in a slightly increased laser amplitude and energy than expected.

namespace picongpu

namespace fields

Typedefs

using Solver = maxwellSolver::Yee
FieldSolver.

Field Solver Selection (note <> for some solvers):
- Yee : Standard Yee solver approximating derivatives with respect to time and space by second order finite differences.
- Lehe<>: Num. Cherenkov free field solver in a chosen direction
- ArbitraryOrderFDTD<4>: Solver using 4 neighbors to each direction to approximate *spatial* derivatives by finite differences. The number of neighbors can be changed from 4 to any positive, integer number. The order of the solver will be twice the number of neighbors in each direction. Yee's method is a special case of this using one neighbor to each direction.
- None: disable the vacuum update of E and B

fieldAbsorber.param

Configure the field absorber parameters.

Field absorber type is set by command-line option fieldAbsorber.

namespace picongpu

namespace fields

namespace absorber

Variables

constexpr uint32_t **THICKNESS** = 12

constexpr uint32_t picongpu::fields::absorber::NUM_CELLS[3][2]= {
Thickness of the absorbing layer, in number of cells.

This setting applies to applies for all absorber kinds. The absorber layer is located inside the global simulation area, near the outer borders. Setting size to 0 results in disabling absorption at the corresponding boundary. Note that for non-absorbing boundaries the actual thickness will be 0 anyways. There are no requirements on thickness being a multiple of the supercell size.

For PML the recommended thickness is between 6 and 16 cells. For the exponential damping it is 32.

Unit: number of cells.

namespace exponential
Settings for the Exponential absorber.

Variables

constexpr float_X picongpu::fields::absorber::exponential::STRENGTH[3][2]=
Define the strength of the absorber for all directions.

Elements corredponding to non-absorber borders will have no effect.

Unit: none

namespace pml
Settings for the Pml absorber.

These parameters can generally be left with default values. For more details on the meaning of the parameters, refer to the following references. J.A. Roden, S.D. Gedney. Convolution PML (CPML): An efficient FDTD implementation of the CFS - PML for arbitrary media. Microwave and optical technology letters. 27 (5), 334-339 (2000). A. Taflove, S.C. Hagness. Computational Electrodynamics. The Finite-Difference Time-Domain Method. Third Edition. Artech house, Boston (2005), referred to as [Taflove, Hagness].

Variables

constexpr float_64 **SIGMA_KAPPA_GRADING_ORDER** = 4.0
Order of polynomial grading for artificial electric conductivity and stretching coefficient.

The conductivity (sigma) is polynomially scaling from 0 at the internal border of PML to the maximum value (defined below) at the external border. The stretching coefficient (kappa) scales from 1 to the corresponding maximum value (defined below) with the same polynomial. The grading is given in [Taflove, Hagness], eq. (7.60a, b), with the order denoted 'm'. Must be >= 0. Normally between 3 and 4, not required to be integer. Unitless.

constexpr float_64 **SIGMA_OPT_SI**[3] = {0.8 * (*SIGMA_KAPPA_GRADING_ORDER* + 1.0) / (*SI*::*Z0_SI*

constexpr float_64 **SIGMA_OPT_MULTIPLIER** = 1.0

constexpr float_64 **SIGMA_MAX_SI**[3] = {*SIGMA_OPT_SI*[0] * *SIGMA_OPT_MULTIPLIER*, , }
Max value of artificial electric conductivity in PML.

Components correspond to directions: element 0 corresponds to absorption along x direction, 1 = y, 2 = z. Grading is described in comments for SIGMA_KAPPA_GRADING_ORDER. Too small values lead to significant reflections from the external border, too large - to reflections due to discretization errors. Artificial magnetic permeability will be chosen to perfectly match this. Must be >= 0. Normally between 0.7 * SIGMA_OPT_SI and 1.1 * SIGMA_OPT_SI. Unit: siemens / m.

constexpr float_64 **KAPPA_MAX**[3] = {1.0, , }
Max value of coordinate stretching coefficient in PML.

Components correspond to directions: element 0 corresponds to absorption along x direction, 1 = y, 2 = z. Grading is described in comments for SIGMA_KAPPA_GRADING_ORDER. Must be >= 1. For relatively homogeneous

domains 1.0 is a reasonable value. Highly elongated domains can have better absorption with values between 7.0 and 20.0, for example, see section 7.11.2 in [Taflove, Hagness]. Unitless.

constexpr float_64 **ALPHA_GRADING_ORDER** = 1.0
Order of polynomial grading for complex frequency shift.

The complex frequency shift (alpha) is polynomially downscaling from the maximum value (defined below) at the internal border of PML to 0 at the external border. The grading is given in [Taflove, Hagness], eq. (7.79), with the order denoted 'm_a'. Must be >= 0. Normally values are around 1.0. Unitless.

constexpr float_64 **ALPHA_MAX_SI**[3] = {0.2, , }
Complex frequency shift in PML.

Components correspond to directions: element 0 corresponds to absorption along x direction, 1 = y, 2 = z. Setting it to 0 will make PML behave as uniaxial PML. Setting it to a positive value helps to attenuate evanescent modes, but can degrade absorption of propagating modes, as described in section 7.7 and 7.11.3 in [Taflove, Hagness]. Must be >= 0. Normally values are 0 or between 0.15 and 0.3. Unit: siemens / m.

laser.param

Configure laser profiles.

All laser propagate in y direction.

Available profiles:

- None : no laser init
- GaussianBeam : Gaussian beam (focusing)
- PulseFrontTilt : Gaussian beam with a tilted pulse envelope in 'x' direction
- PlaneWave : a plane wave (Gaussian in time)
- Wavepacket : wavepacket (Gaussian in time and space, not focusing)
- Polynom : a polynomial laser envelope
- ExpRampWithPrepulse : wavepacket with exponential upramps and prepulse

In the end, this file needs to define a `Selected` class in namespace `picongpu::fields::laserProfiles`. A typical profile consists of a laser profile class and its parameters. For example:

```
using Selected = GaussianBeam< GaussianBeamParam >;
```

namespace picongpu

namespace fields

namespace laserProfiles

Typedefs

using Selected = *None*<>
currently selected laser profile

struct ExpRampWithPrepulseParam
Based on a wavepacket with Gaussian spatial envelope.

and the following temporal shape: A Gaussian peak (optionally lengthened by a plateau) is preceded by two pieces of exponential preramps, defined by 3 (time, intensity)- -points. The first two points get connected by an exponential, the 2nd and 3rd point are connected by another exponential, which is then extrapolated to the peak. The Gaussian is added everywhere, but typically contributes significantly only near the peak. It is advisable to set the third point far enough from the plateau (approx 3*FWHM), then the contribution from the Gaussian is negligible there, and the intensity can be set as measured from the laser profile. Optionally a Gaussian prepulse can be added, given by the parameters of the relative intensity and time point. The time of the prepulse and the three preramp points are given in SI, the intensities are given as multiples of the peak intensity.

Public Types

enum PolarisationType
Available polarisation types.

Values:

LINEAR_X = 1u

LINEAR_Z = 2u

CIRCULAR = 4u

Public Static Attributes

constexpr float_X **INT_RATIO_PREPULSE** = 0.

constexpr float_X **INT_RATIO_POINT_1** = 1.e-8

constexpr float_X **INT_RATIO_POINT_2** = 1.e-4

constexpr float_X **INT_RATIO_POINT_3** = 1.e-4

constexpr float_64 **TIME_PREPULSE_SI** = -950.0e-15

constexpr float_64 **TIME_PEAKPULSE_SI** = 0.0e-15

constexpr float_64 **TIME_POINT_1_SI** = -1000.0e-15

constexpr float_64 **TIME_POINT_2_SI** = -300.0e-15

constexpr float_64 **TIME_POINT_3_SI** = -100.0e-15

constexpr float_64 **WAVE_LENGTH_SI** = 0.8e-6
unit: meter

constexpr float_64 **UNITCONV_A0_to_Amplitude_SI** = -2.0 * *PI* / *WAVE_LENGTH_SI* * *picongpu*::
UNITCONV.

constexpr float_64 **_A0** = 20.
unit: W / m^2

unit: none

constexpr float_64 **AMPLITUDE_SI** = *_A0* * *UNITCONV_A0_to_Amplitude_SI*
unit: Volt /meter

constexpr float_64 **LASER_NOFOCUS_CONSTANT_SI** = 0.0 * *WAVE_LENGTH_SI* / *picongpu*::*SI*::*SPE*
unit: Volt /meter

The profile of the test Lasers 0 and 2 can be stretched by a constant area between the up and downramp unit: seconds

constexpr float_64 **PULSE_LENGTH_SI** = 3.0e-14 / 2.35482
Pulse length: sigma of std.

gauss for intensity (E^2) PULSE_LENGTH_SI = FWHM_of_Intensity / [2*sqrt{ 2* ln(2) }] [2.354820045] Info: FWHM_of_Intensity = FWHM_Illumination = what a experimentalist calls "pulse duration" unit: seconds (1 sigma)

constexpr float_64 **W0_X_SI** = 2.5 * *WAVE_LENGTH_SI*
beam waist: distance from the axis where the pulse intensity (E^2) decreases to its 1/e^2-th part, WO_X_SI is this distance in x-direction W0_Z_SI is this distance in z-direction if both values are equal, the laser has a circular shape in x-z W0_SI = FWHM_of_Intensity / sqrt{ 2* ln(2) } [1.17741] unit: meter

constexpr float_64 **W0_Z_SI** = *W0_X_SI*

constexpr float_64 **RAMP_INIT** = 16.0
The laser pulse will be initialized half of PULSE_INIT times of the PULSE_LENGTH before plateau and half at the end of the plateau unit: none.

constexpr uint32_t **initPlaneY** = 0
cell from top where the laser is initialized

if `initPlaneY == 0` than the absorber are disabled. if `initPlaneY > absorbercells negative Y` the negative absorber in y direction is enabled

valid ranges:
- initPlaneY == 0
- absorber cells negative Y < initPlaneY < cells in y direction of the top gpu

constexpr float_X **LASER_PHASE** = 0.0
laser phase shift (no shift: 0.0)

sin(omega*time + laser_phase): starts with phase=0 at center > E-field=0 at center

unit: rad, periodic in 2*pi

constexpr *PolarisationType* **Polarisation** = *LINEAR_X*
Polarization selection.

struct GaussianBeamParam

Public Types

enum PolarisationType
Available polarisation types.

Values:

LINEAR_X = 1u

LINEAR_Z = 2u

CIRCULAR = 4u

using LAGUERREMODES_t = *gaussianBeam*::LAGUERREMODES_t

Public Static Attributes

constexpr float_64 **WAVE_LENGTH_SI** = 0.8e-6
unit: meter

constexpr float_64 **UNITCONV_A0_to_Amplitude_SI** = -2.0 * *PI* / *WAVE_LENGTH_SI* * *picongpu*::
Convert the normalized laser strength parameter a0 to Volt per meter.

constexpr float_64 **AMPLITUDE_SI** = 1.738e13
unit: W / m^2

unit: none unit: Volt / meter unit: Volt / meter

constexpr float_64 **PULSE_LENGTH_SI** = 10.615e-15 / 4.0
Pulse length: sigma of std.

gauss for intensity (E^2) PULSE_LENGTH_SI = FWHM_of_Intensity / [2*sqrt{ 2* ln(2) }] [2.354820045] Info: FWHM_of_Intensity = FWHM_Illumination = what a experimentalist calls "pulse duration"

unit: seconds (1 sigma)

constexpr float_64 **W0_SI** = 5.0e-6 / 1.17741
beam waist: distance from the axis where the pulse intensity (E^2) decreases to its 1/e^2-th part, at the focus position of the laser W0_SI = FWHM_of_Intensity / sqrt{ 2* ln(2) } [1.17741]

unit: meter

constexpr float_64 **FOCUS_POS_SI** = 4.62e-5
the distance to the laser focus in y-direction unit: meter

constexpr float_64 **PULSE_INIT** = 20.0
The laser pulse will be initialized PULSE_INIT times of the PULSE_LENGTH.

unit: none

constexpr uint32_t **initPlaneY** = 0
cell from top where the laser is initialized

if `initPlaneY == 0` than the absorber are disabled. if `initPlaneY > absorbercells negative Y` the negative absorber in y direction is enabled

valid ranges:
- initPlaneY == 0
- absorber cells negative Y < initPlaneY < cells in y direction of the top gpu

constexpr float_X **LASER_PHASE** = 0.0
laser phase shift (no shift: 0.0)

sin(omega*time + laser_phase): starts with phase=0 at center > E-field=0 at center

unit: rad, periodic in 2*pi

constexpr uint32_t **MODENUMBER** = *gaussianBeam::MODENUMBER*

constexpr *PolarisationType* **Polarisation** = *CIRCULAR*
Polarization selection.

struct PlaneWaveParam

Public Types

enum PolarisationType
Available polarization types.

Values:

LINEAR_X = 1u

LINEAR_Z = 2u

CIRCULAR = 4u

Public Static Attributes

constexpr float_64 **WAVE_LENGTH_SI** = 0.8e-6
unit: meter

constexpr float_64 **UNITCONV_A0_to_Amplitude_SI** = -2.0 * *PI* / *WAVE_LENGTH_SI* * *picongpu*::
Convert the normalized laser strength parameter a0 to Volt per meter.

constexpr float_64 **_A0** = 1.5
unit: W / m^2

unit: none

constexpr float_64 **AMPLITUDE_SI** = *_A0* * *UNITCONV_A0_to_Amplitude_SI*
unit: Volt / meter

constexpr float_64 **LASER_NOFOCUS_CONSTANT_SI** = 13.34e-15
unit: Volt / meter

The profile of the test Lasers 0 and 2 can be stretched by a constant area between the up and downramp unit: seconds

constexpr float_64 **PULSE_LENGTH_SI** = 10.615e-15 / 4.0
Pulse length: sigma of std.

gauss for intensity (E^2) PULSE_LENGTH_SI = FWHM_of_Intensity / [2*sqrt{ 2* ln(2) }] [2.354820045] Info: FWHM_of_Intensity = FWHM_Illumination = what a experimentalist calls "pulse duration" unit: seconds (1 sigma)

constexpr uint32_t **initPlaneY** = 0
cell from top where the laser is initialized

if `initPlaneY == 0` than the absorber are disabled. if `initPlaneY > absorbercells negative Y` the negative absorber in y direction is enabled

valid ranges:
- initPlaneY == 0
- absorber cells negative Y < initPlaneY < cells in y direction of the top gpu

constexpr float_64 **RAMP_INIT** = 20.6146
The laser pulse will be initialized half of PULSE_INIT times of the PULSE_LENGTH before and after the plateau unit: none.

constexpr float_X **LASER_PHASE** = 0.0
laser phase shift (no shift: 0.0)

sin(omega*time + laser_phase): starts with phase=0 at center > E-field=0 at center

unit: rad, periodic in 2*pi

constexpr *PolarisationType* **Polarisation** = *LINEAR_X*
Polarization selection.

struct PolynomParam
Based on a wavepacket with Gaussian spatial envelope.

Wavepacket with a polynomial temporal intensity shape.

Public Types

enum PolarisationType
Available polarization types.

Values:

LINEAR_X = 1u

LINEAR_Z = 2u

CIRCULAR = 4u

Public Static Attributes

constexpr float_64 **WAVE_LENGTH_SI** = 0.8e-6
unit: meter

constexpr float_64 **UNITCONV_A0_to_Amplitude_SI** = -2.0 * *PI* / *WAVE_LENGTH_SI* * *picongpu*::
Convert the normalized laser strength parameter a0 to Volt per meter.

constexpr float_64 **AMPLITUDE_SI** = 1.738e13
unit: W / m^2

unit: none unit: Volt / meter unit: Volt / meter

constexpr float_64 **LASER_NOFOCUS_CONSTANT_SI** = 13.34e-15
The profile of the test Lasers 0 and 2 can be stretched by a constant area between the up and downramp unit: seconds.

constexpr float_64 **PULSE_LENGTH_SI** = 10.615e-15 / 4.0
Pulse length: sigma of std.

gauss for intensity (E^2) PULSE_LENGTH_SI = FWHM_of_Intensity / [2*sqrt{ 2* ln(2) }] [2.354820045] Info: FWHM_of_Intensity = FWHM_Illumination = what a experimentalist calls "pulse duration" unit: seconds (1 sigma)

constexpr float_64 **W0_X_SI** = 4.246e-6
beam waist: distance from the axis where the pulse intensity (E^2) decreases to its 1/e^2-th part, at the focus position of the laser unit: meter

constexpr float_64 **W0_Z_SI** = *W0_X_SI*

constexpr uint32_t **initPlaneY** = 0
cell from top where the laser is initialized

if `initPlaneY == 0` than the absorber are disabled. if `initPlaneY > absorbercells negative Y` the negative absorber in y direction is enabled

valid ranges:
- initPlaneY == 0
- absorber cells negative Y < initPlaneY < cells in y direction of the top gpu

constexpr float_64 **PULSE_INIT** = 20.0
The laser pulse will be initialized PULSE_INIT times of the PULSE_LENGTH.

unit: none

constexpr float_X **LASER_PHASE** = 0.0
laser phase shift (no shift: 0.0)

sin(omega*time + laser_phase): starts with phase=0 at center > E-field=0 at center

unit: rad, periodic in 2*pi

constexpr *PolarisationType* **Polarisation** = *LINEAR_X*
Polarization selection.

struct PulseFrontTiltParam

Public Types

enum PolarisationType
Available polarisation types.

Values:

LINEAR_X = 1u

LINEAR_Z = 2u

CIRCULAR = 4u

Public Static Attributes

constexpr float_64 **WAVE_LENGTH_SI** = 0.8e-6
unit: meter

constexpr float_64 **UNITCONV_A0_to_Amplitude_SI** = -2.0 * *PI* / *WAVE_LENGTH_SI* * *picongpu*::
Convert the normalized laser strength parameter a0 to Volt per meter.

constexpr float_64 **AMPLITUDE_SI** = 1.738e13
unit: W / m^2

unit: none unit: Volt / meter unit: Volt / meter

constexpr float_64 **PULSE_LENGTH_SI** = 10.615e-15 / 4.0
Pulse length: sigma of std.

gauss for intensity (E^2) PULSE_LENGTH_SI = FWHM_of_Intensity / [2*sqrt{ 2* ln(2) }] [2.354820045] Info: FWHM_of_Intensity = FWHM_Illumination = what a experimentalist calls "pulse duration"

unit: seconds (1 sigma)

constexpr float_64 **W0_SI** = 5.0e-6 / 1.17741
beam waist: distance from the axis where the pulse intensity (E^2) decreases to its 1/e^2-th part, at the focus position of the laser W0_SI = FWHM_of_Intensity / sqrt{ 2* ln(2) } [1.17741]

unit: meter

constexpr float_64 **FOCUS_POS_SI** = 4.62e-5
the distance to the laser focus in y-direction unit: meter

constexpr float_64 **TILT_X_SI** = 0.0
the tilt angle between laser propagation in y-direction and laser axis in x-direction (0 degree == no tilt) unit: degree

constexpr float_64 **PULSE_INIT** = 20.0
The laser pulse will be initialized PULSE_INIT times of the PULSE_LENGTH.

unit: none

constexpr uint32_t **initPlaneY** = 0
cell from top where the laser is initialized

if `initPlaneY == 0` than the absorber are disabled. if `initPlaneY > absorbercells negative Y` the negative absorber in y direction is enabled

valid ranges:
- initPlaneY == 0
- absorber cells negative Y < initPlaneY < cells in y direction of the top gpu

constexpr float_X **LASER_PHASE** = 0.0
laser phase shift (no shift: 0.0)

sin(omega*time + laser_phase): starts with phase=0 at center > E-field=0 at center

unit: rad, periodic in 2*pi

constexpr *PolarisationType* **Polarisation** = *CIRCULAR*
Polarization selection.

struct WavepacketParam

Public Types

enum PolarisationType
Available polarisation types.

Values:

LINEAR_X = 1u

LINEAR_Z = 2u

CIRCULAR = 4u

Public Static Attributes

constexpr float_64 **WAVE_LENGTH_SI** = 0.8e-6
unit: meter

constexpr float_64 **UNITCONV_A0_to_Amplitude_SI** = -2.0 * *PI* / *WAVE_LENGTH_SI* * *picongpu*::
Convert the normalized laser strength parameter a0 to Volt per meter.

constexpr float_64 **AMPLITUDE_SI** = 1.738e13
unit: W / m^2

unit: none unit: Volt / meter unit: Volt / meter

constexpr float_64 **LASER_NOFOCUS_CONSTANT_SI** = 7.0 * *WAVE_LENGTH_SI* / *picongpu*::*SI*::*SPEE*
The profile of the test Lasers 0 and 2 can be stretched by a constant area between the up and downramp unit: seconds.

constexpr float_64 **PULSE_LENGTH_SI** = 10.615e-15 / 4.0
Pulse length: sigma of std.

gauss for intensity (E^2) PULSE_LENGTH_SI = FWHM_of_Intensity / [2*sqrt{ 2* ln(2) }] [2.354820045] Info: FWHM_of_Intensity = FWHM_Illumination = what a experimentalist calls "pulse duration"

unit: seconds (1 sigma)

constexpr float_64 **W0_X_SI** = 4.246e-6
beam waist: distance from the axis where the pulse intensity (E^2) decreases to its 1/e^2-th part, at the focus position of the laser W0_SI = FWHM_of_Intensity / sqrt{ 2* ln(2) } [1.17741]

unit: meter

constexpr float_64 **W0_Z_SI** = *W0_X_SI*

constexpr float_64 **PULSE_INIT** = 20.0
The laser pulse will be initialized PULSE_INIT times of the PULSE_LENGTH.

unit: none

constexpr uint32_t **initPlaneY** = 0
cell from top where the laser is initialized

if `initPlaneY == 0` than the absorber are disabled. if `initPlaneY > absorbercells negative Y` the negative absorber in y direction is enabled

valid ranges:
- initPlaneY == 0
- absorber cells negative Y < initPlaneY < cells in y direction of the top gpu

constexpr float_X **LASER_PHASE** = 0.0
laser phase shift (no shift: 0.0)

sin(omega*time + laser_phase): starts with phase=0 at center > E-field=0 at center

unit: rad, periodic in 2*pi

constexpr *PolarisationType* **Polarisation** = *LINEAR_X*
Polarization selection.

namespace gaussianBeam

Functions

picongpu::fields::laserProfiles::gaussianBeam::PMACC_CONST_VECTOR(float_X,

Variables

constexpr uint32_t **MODENUMBER** = 0
Use only the 0th Laguerremode for a standard Gaussian.

List of available laser profiles.

Laser Profiles

Gaussian Beam

template<typename **T_Params**>
struct GaussianBeam : **public** *picongpu*::*fields*::*laserProfiles*::*gaussianBeam*::Unitless<*T_Params*>
Gaussian Beam laser profile with finite pulse length.

Template Parameters

- T_Params: class parameter to configure the Gaussian Beam profile, see members of gaussianBeam::default::GaussianBeamParam for required members

```
                    //! Use only the 0th Laguerremode for a standard Gaussian
                    static constexpr uint32_t MODENUMBER = 0;
                    PMACC_CONST_VECTOR(float_X, MODENUMBER + 1, LAGUERREMODES, 1.
↪0);
                    // This is just an example for a more complicated set of␣
↪Laguerre modes
                    // constexpr uint32_t MODENUMBER = 12;
                    // PMACC_CONST_VECTOR(float_X, MODENUMBER + 1, LAGUERREMODES, -
↪1.0, 0.0300519, 0.319461, -0.23783,
                    // 0.0954839, 0.0318653, -0.144547, 0.0249208, -0.111989, 0.
↪0434385, -0.030038, -0.00896321,
                    // -0.0160788);

                    struct GaussianBeamParam
                    {
                        /** unit: meter */
                        static constexpr float_64 WAVE_LENGTH_SI = 0.8e-6;

                        /** Convert the normalized laser strength parameter a0 to␣
↪Volt per meter */
                        static constexpr float_64 UNITCONV_A0_to_Amplitude_SI = -2.
↪0 * PI / WAVE_LENGTH_SI
                            * ::picongpu::SI::ELECTRON_MASS_SI *␣
↪::picongpu::SI::SPEED_OF_LIGHT_SI
                            * ::picongpu::SI::SPEED_OF_LIGHT_SI /␣
↪::picongpu::SI::ELECTRON_CHARGE_SI;

                        /** unit: W / m^2 */
```

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```
                        // calculate: _A0 = 8.549297e-6 * sqrt( Intensity[W/m^2] )␣
↪* wavelength[m] (linearly polarized)

                        /** unit: none */
                        // static constexpr float_64 _A0  = 1.5;

                        /** unit: Volt / meter */
                        // static constexpr float_64 AMPLITUDE_SI = _A0 * UNITCONV_
↪A0_to_Amplitude_SI;

                        /** unit: Volt / meter */
                        static constexpr float_64 AMPLITUDE_SI = 1.738e13;

                        /** Pulse length: sigma of std. gauss for intensity (E^2)
                         *  PULSE_LENGTH_SI = FWHM_of_Intensity   / [ 2*sqrt{ 2*␣
↪ln(2) } ]
                         *                                          [    2.
↪354820045     ]
                         *  Info:             FWHM_of_Intensity = FWHM_Illumination
                         *                      = what a experimentalist calls
↪"pulse duration"
                         *
                         *  unit: seconds (1 sigma) */
                        static constexpr float_64 PULSE_LENGTH_SI = 10.615e-15 / 4.
↪0;

                        /** beam waist: distance from the axis where the pulse␣
↪intensity (E^2)
                         *              decreases to its 1/e^2-th part,
                         *              at the focus position of the laser
                         * W0_SI = FWHM_of_Intensity / sqrt{ 2* ln(2) }
                         *                               [   1.17741    ]
                         *
                         *  unit: meter */
                        static constexpr float_64 W0_SI = 5.0e-6 / 1.17741;
                        /** the distance to the laser focus in y-direction
                         *  unit: meter */
                        static constexpr float_64 FOCUS_POS_SI = 4.62e-5;

                        /** The laser pulse will be initialized PULSE_INIT times␣
↪of the PULSE_LENGTH
                         *
                         *  unit: none */
                        static constexpr float_64 PULSE_INIT = 20.0;

                        /** cell from top where the laser is initialized
                         *
                         * if `initPlaneY == 0` than the absorber are disabled.
                         * if `initPlaneY > absorbercells negative Y` the negative␣
↪absorber in y
                         * direction is enabled
                         *
                         * valid ranges:
                         *   - initPlaneY == 0
                         *   - absorber cells negative Y < initPlaneY < cells in y␣
↪direction of the top gpu
                         */
                        static constexpr uint32_t initPlaneY = 0;

                        /** laser phase shift (no shift: 0.0)
                         *
```

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```
                         * sin(omega*time + laser_phase): starts with phase=0 at␣
↪center --> E-field=0 at center
                         *
                         * unit: rad, periodic in 2*pi
                         */
                        static constexpr float_X LASER_PHASE = 0.0;

                        using LAGUERREMODES_t = defaults::LAGUERREMODES_t;
                        static constexpr uint32_t MODENUMBER =␣
↪defaults::MODENUMBER;

                        /** Available polarisation types
                         */
                        enum PolarisationType
                        {
                            LINEAR_X = 1u,
                            LINEAR_Z = 2u,
                            CIRCULAR = 4u,
                        };
```

Gaussian Beam with Pulse Front Tilt

template<typename **T_Params**>
struct PulseFrontTilt : **public** *picongpu*::*fields*::*laserProfiles*::pulseFrontTilt::Unitless<*T_Params*>
Gaussian Beam laser profile with titled pulse front.

Template Parameters

- T_Params: class parameter to configure the Gaussian Beam with pulse front titlt, see members of pulseFrontTilt::defaults::PulseFrontTiltParam for required members

```
                    struct PulseFrontTiltParam
                    {
                        /** unit: meter */
                        static constexpr float_64 WAVE_LENGTH_SI = 0.8e-6;

                        /** Convert the normalized laser strength parameter a0 to␣
↪Volt per meter */
                        static constexpr float_64 UNITCONV_A0_to_Amplitude_SI = -2.
↪0 * PI / WAVE_LENGTH_SI
                            * ::picongpu::SI::ELECTRON_MASS_SI *␣
↪::picongpu::SI::SPEED_OF_LIGHT_SI
                            * ::picongpu::SI::SPEED_OF_LIGHT_SI /␣
↪::picongpu::SI::ELECTRON_CHARGE_SI;

                        /** unit: W / m^2 */
                        // calculate: _A0 = 8.549297e-6 * sqrt( Intensity[W/m^2] )␣
↪* wavelength[m] (linearly polarized)

                        /** unit: none */
                        // static constexpr float_64 _A0  = 1.5;

                        /** unit: Volt / meter */
                        // static constexpr float_64 AMPLITUDE_SI = _A0 * UNITCONV_
↪A0_to_Amplitude_SI;

                        /** unit: Volt / meter */
                        static constexpr float_64 AMPLITUDE_SI = 1.738e13;
```

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```
                        /** Pulse length: sigma of std. gauss for intensity (E^2)
                         *  PULSE_LENGTH_SI = FWHM_of_Intensity   / [ 2*sqrt{ 2*␣
↪ln(2) } ]
                         *                                          [    2.
↪354820045     ]
                         *  Info:             FWHM_of_Intensity = FWHM_Illumination
                         *                      = what a experimentalist calls
↪"pulse duration"
                         *
                         *  unit: seconds (1 sigma) */
                        static constexpr float_64 PULSE_LENGTH_SI = 10.615e-15 / 4.
↪0;

                        /** beam waist: distance from the axis where the pulse␣
↪intensity (E^2)
                         *              decreases to its 1/e^2-th part,
                         *              at the focus position of the laser
                         * W0_SI = FWHM_of_Intensity / sqrt{ 2* ln(2) }
                         *                             [   1.17741    ]
                         *
                         *  unit: meter */
                        static constexpr float_64 W0_SI = 5.0e-6 / 1.17741;

                        /** the distance to the laser focus in y-direction
                         *  unit: meter */
                        static constexpr float_64 FOCUS_POS_SI = 4.62e-5;

                        /** the tilt angle between laser propagation in y-
↪direction and laser axis in
                         *  x-direction (0 degree == no tilt)
                         *  unit: degree */
                        static constexpr float_64 TILT_X_SI = 0.0;

                        /** The laser pulse will be initialized PULSE_INIT times␣
↪of the PULSE_LENGTH
                         *
                         *  unit: none */
                        static constexpr float_64 PULSE_INIT = 20.0;

                        /** cell from top where the laser is initialized
                         *
                         * if `initPlaneY == 0` than the absorber are disabled.
                         * if `initPlaneY > absorbercells negative Y` the negative␣
↪absorber in y
                         * direction is enabled
                         *
                         * valid ranges:
                         *   - initPlaneY == 0
                         *   - absorber cells negative Y < initPlaneY < cells in y␣
↪direction of the top gpu
                         */
                        static constexpr uint32_t initPlaneY = 0;

                        /** laser phase shift (no shift: 0.0)
                         *
                         * sin(omega*time + laser_phase): starts with phase=0 at␣
↪center --> E-field=0 at center
                         *
                         * unit: rad, periodic in 2*pi
                         */
                        static constexpr float_X LASER_PHASE = 0.0;
```

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```
                        //! Available polarisation types
                        enum PolarisationType
                        {
                            LINEAR_X = 1u,
                            LINEAR_Z = 2u,
                            CIRCULAR = 4u,
                        };

                        /** Polarization selection
                         */
```

Wavepacket

template<typename **T_Params**>
struct Wavepacket : **public** *picongpu*::*fields*::*laserProfiles*::wavepacket::Unitless<*T_Params*>
Wavepacket with Gaussian spatial and temporal envelope.

Template Parameters

- T_Params: class parameter to configure the *Wavepacket* profile, see members of wavepacket::defaults::WavepacketParam for required members

```
                    struct WavepacketParam
                    {
                        /** unit: meter */
                        static constexpr float_64 WAVE_LENGTH_SI = 0.8e-6;

                        /** Convert the normalized laser strength parameter a0 to␣
↪Volt per meter */
                        static constexpr float_64 UNITCONV_A0_to_Amplitude_SI = -2.
↪0 * PI / WAVE_LENGTH_SI
                            * ::picongpu::SI::ELECTRON_MASS_SI *␣
↪::picongpu::SI::SPEED_OF_LIGHT_SI
                            * ::picongpu::SI::SPEED_OF_LIGHT_SI /␣
↪::picongpu::SI::ELECTRON_CHARGE_SI;

                        /** unit: W / m^2 */
                        // calculate: _A0 = 8.549297e-6 * sqrt( Intensity[W/m^2] )␣
↪* wavelength[m] (linearly polarized)

                        /** unit: none */
                        // static constexpr float_64 _A0  = 1.5;

                        /** unit: Volt / meter */
                        // static constexpr float_64 AMPLITUDE_SI = _A0 * UNITCONV_
↪A0_to_Amplitude_SI;

                        /** unit: Volt / meter */
                        static constexpr float_64 AMPLITUDE_SI = 1.738e13;

                        /** Stretch temporal profile by a constant plateau between␣
↪the up and downramp
                         *  unit: seconds */
                        static constexpr float_64 LASER_NOFOCUS_CONSTANT_SI
                            = 7.0 * WAVE_LENGTH_SI / ::picongpu::SI::SPEED_OF_
↪LIGHT_SI;

                        /** Pulse length: sigma of std. gauss for intensity (E^2)
```

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```
                         *  PULSE_LENGTH_SI = FWHM_of_Intensity   / [ 2*sqrt{ 2*ln(2) } ]
                         *                                          [    2.354820045     ]
                         *  Info:             FWHM_of_Intensity = FWHM_Illumination
                         *                      = what a experimentalist calls "pulse duration"
                         *
                         *  unit: seconds (1 sigma) */
                        static constexpr float_64 PULSE_LENGTH_SI = 10.615e-15 / 4.0;

                        /** beam waist: distance from the axis where the pulse intensity (E^2)
                         *              decreases to its 1/e^2-th part,
                         *              at the focus position of the laser
                         * W0_SI = FWHM_of_Intensity / sqrt{ 2* ln(2) }
                         *                             [   1.17741    ]
                         *
                         *  unit: meter */
                        static constexpr float_64 W0_X_SI = 4.246e-6;
                        static constexpr float_64 W0_Z_SI = W0_X_SI;

                        /** The laser pulse will be initialized PULSE_INIT times of the PULSE_LENGTH
                         *
                         *  unit: none */
                        static constexpr float_64 PULSE_INIT = 20.0;

                        /** cell from top where the laser is initialized
                         *
                         * if `initPlaneY == 0` than the absorber are disabled.
                         * if `initPlaneY > absorbercells negative Y` the negative absorber in y
                         * direction is enabled
                         *
                         * valid ranges:
                         *   - initPlaneY == 0
                         *   - absorber cells negative Y < initPlaneY < cells in y direction of the top gpu
                         */
                        static constexpr uint32_t initPlaneY = 0;

                        /** laser phase shift (no shift: 0.0)
                         *
                         * sin(omega*time + laser_phase): starts with phase=0 at center --> E-field=0 at center
                         *
                         * unit: rad, periodic in 2*pi
                         */
                        static constexpr float_X LASER_PHASE = 0.0;

                        /** Available polarisation types
                         */
                        enum PolarisationType
                        {
                            LINEAR_X = 1u,
                            LINEAR_Z = 2u,
                            CIRCULAR = 4u,
                        };
                        /** Polarization selection
```

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```
                                */
```

Wavepacket with Exponential Ramp and Prepulse

template<typename **T_Params**>
struct ExpRampWithPrepulse : **public** *picongpu*::*fields*::*laserProfiles*::expRampWithPrepulse::Unitless<*T_Params*>

Wavepacket with spatial Gaussian envelope and adjustable temporal shape.

Allows defining a prepulse and two regions of exponential preramp with independent slopes. The definition works by specifying three (t, intensity)- points, where time is counted from the very beginning in SI and the intensity (yes, intensity, not amplitude) is given in multiples of the main peak.

Be careful - problematic for few cycle pulses. Thought the rest is cloned from laserWavepacket, the correctionFactor is not included (this made a correction to the laser phase, which is necessary for very short pulses, since otherwise a test particle is, after the laser pulse has passed, not returned to immobility, as it should). Since the analytical solution is only implemented for the Gaussian regime, and we have mostly exponential regimes here, it was not retained here.

A Gaussian peak (optionally lengthened by a plateau) is preceded by two pieces of exponential preramps, defined by 3 (time, intensity)- -points.

The first two points get connected by an exponential, the 2nd and 3rd point are connected by another exponential, which is then extrapolated to the peak. The Gaussian is added everywhere, but typically contributes significantly only near the peak. It is advisable to set the third point far enough from the plateau (approx 3*FWHM), then the contribution from the Gaussian is negligible there, and the intensity can be set as measured from the laser profile.

Optionally a Gaussian prepulse can be added, given by the parameters of the relative intensity and time point. The time of the prepulse and the three preramp points are given in SI, the intensities are given as multiples of the peak intensity.

Template Parameters

- `T_Params`: class parameter to configure the Gaussian Beam profile, see members of expRampWithPrepulse::defaults::ExpRampWithPrepulseParam for required members

```
                    struct ExpRampWithPrepulseParam
                    {
                        // Intensities of prepulse and exponential preramp
                        static constexpr float_X INT_RATIO_PREPULSE = 0.;
                        static constexpr float_X INT_RATIO_POINT_1 = 1.e-8;
                        static constexpr float_X INT_RATIO_POINT_2 = 1.e-4;
                        static constexpr float_X INT_RATIO_POINT_3 = 1.e-4;

                        // time-positions of prepulse and preramps points
                        static constexpr float_64 TIME_PREPULSE_SI = -950.0e-15;
                        static constexpr float_64 TIME_PEAKPULSE_SI = 0.0e-15;
                        static constexpr float_64 TIME_POINT_1_SI = -1000.0e-15;
                        static constexpr float_64 TIME_POINT_2_SI = -300.0e-15;
                        static constexpr float_64 TIME_POINT_3_SI = -100.0e-15;

                        /** unit: meter */
                        static constexpr float_64 WAVE_LENGTH_SI = 0.8e-6;

                        /** UNITCONV */
                        static constexpr float_64 UNITCONV_A0_to_Amplitude_SI = -2.
↪0 * PI / WAVE_LENGTH_SI
                                * ::picongpu::SI::ELECTRON_MASS_SI *␣
↪::picongpu::SI::SPEED_OF_LIGHT_SI
```

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```
                            * ::picongpu::SI::SPEED_OF_LIGHT_SI /␣
↪::picongpu::SI::ELECTRON_CHARGE_SI;

                        /** unit: W / m^2 */
                        // calculate: _A0 = 8.549297e-6 * sqrt( Intensity[W/m^2] )␣
↪* wavelength[m] (linearly polarized)

                        /** unit: none */
                        static constexpr float_64 _A0 = 20.;

                        /** unit: Volt /meter */
                        static constexpr float_64 AMPLITUDE_SI = _A0 * UNITCONV_A0_
↪to_Amplitude_SI;

                        /** unit: Volt /meter */
                        // constexpr float_64 AMPLITUDE_SI = 1.738e13;

                        /** Stretch temporal profile by a constant plateau between␣
↪the up and downramp
                         *  unit: seconds */
                        static constexpr float_64 LASER_NOFOCUS_CONSTANT_SI
                            = 0.0 * WAVE_LENGTH_SI / ::picongpu::SI::SPEED_OF_
↪LIGHT_SI;

                        /** Pulse length: sigma of std. gauss for intensity (E^2)
                         *  PULSE_LENGTH_SI = FWHM_of_Intensity   / [ 2*sqrt{ 2*␣
↪ln(2) } ]
                         *                                          [    2.
↪354820045     ]
                         *  Info:             FWHM_of_Intensity = FWHM_Illumination
                         *                      = what a experimentalist calls
↪"pulse duration"
                         *  unit: seconds (1 sigma) */
                        static constexpr float_64 PULSE_LENGTH_SI = 3.0e-14
                            / 2.35482; // half of the time in which E falls to␣
↪half its initial value (then I falls to
                                       // half its value in 15fs, approx 6␣
↪wavelengths). Those are 4.8 wavelenghts.

                        /** beam waist: distance from the axis where the pulse␣
↪intensity (E^2)
                         *              decreases to its 1/e^2-th part,
                         *              W0_X_SI is this distance in x-direction
                         *              W0_Z_SI is this distance in z-direction
                         *              if both values are equal, the laser has a␣
↪circular shape in x-z
                         * W0_SI = FWHM_of_Intensity / sqrt{ 2* ln(2) }
                         *                             [   1.17741    ]
                         *  unit: meter */
                        static constexpr float_64 W0_X_SI = 2.5 * WAVE_LENGTH_SI;
                        static constexpr float_64 W0_Z_SI = W0_X_SI;

                        /** The laser pulse will be initialized half of PULSE_INIT␣
↪times of the PULSE_LENGTH before
                         * plateau and half at the end of the plateau unit: none */
                        static constexpr float_64 RAMP_INIT = 16.0;

                        /** cell from top where the laser is initialized
                         *
                         * if `initPlaneY == 0` than the absorber are disabled.
                         * if `initPlaneY > absorbercells negative Y` the negative␣
↪absorber in y
```

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```
                         * direction is enabled
                         *
                         * valid ranges:
                         *   - initPlaneY == 0
                         *   - absorber cells negative Y < initPlaneY < cells in y␣
↪direction of the top gpu
                         */
                        static constexpr uint32_t initPlaneY = 0;

                        /** laser phase shift (no shift: 0.0)
                         *
                         * sin(omega*time + laser_phase): starts with phase=0 at␣
↪center --> E-field=0 at center
                         *
                         * unit: rad, periodic in 2*pi
                         */
                        static constexpr float_X LASER_PHASE = 0.0;

                        /** Available polarisation types
                         */
                        enum PolarisationType
                        {
                            LINEAR_X = 1u,
                            LINEAR_Z = 2u,
                            CIRCULAR = 4u,
                        };

                        /** Polarization selection
```

Wavepacket with Polynomial Profile

template<typename **T_Params**>
struct Polynom : **public** *picongpu*::*fields*::*laserProfiles*::polynom::Unitless<*T_Params*>

Wavepacket with a polynomial temporal intensity shape.

Based on a wavepacket with Gaussian spatial envelope.

Template Parameters

- T_Params: class parameter to configure the polynomial laser profile, see members of polynom::defaults::PolynomParam for required members

```
                    struct PolynomParam
                    {
                        /** unit: meter */
                        static constexpr float_64 WAVE_LENGTH_SI = 0.8e-6;

                        /** Convert the normalized laser strength parameter a0 to␣
↪Volt per meter */
                        static constexpr float_64 UNITCONV_A0_to_Amplitude_SI = -2.
↪0 * PI / WAVE_LENGTH_SI
                            * ::picongpu::SI::ELECTRON_MASS_SI *␣
↪::picongpu::SI::SPEED_OF_LIGHT_SI
                            * ::picongpu::SI::SPEED_OF_LIGHT_SI /␣
↪::picongpu::SI::ELECTRON_CHARGE_SI;

                        /** unit: W / m^2 */
                        // calculate: _A0 = 8.549297e-6 * sqrt( Intensity[W/m^2] )␣
↪* wavelength[m] (linearly polarized)
```

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```
                        /** unit: none */
                        // static constexpr float_64 _A0  = 1.5;

                        /** unit: Volt / meter */
                        // static constexpr float_64 AMPLITUDE_SI = _A0 * UNITCONV_
↪A0_to_Amplitude_SI;

                        /** unit: Volt / meter */
                        static constexpr float_64 AMPLITUDE_SI = 1.738e13;

                        /** Pulse length: sigma of std. gauss for intensity (E^2)
                         *  PULSE_LENGTH_SI = FWHM_of_Intensity   / [ 2*sqrt{ 2*␣
↪ln(2) } ]
                         *                                          [    2.
↪354820045     ]
                         *  Info:             FWHM_of_Intensity = FWHM_Illumination
                         *                      = what a experimentalist calls
↪"pulse duration"
                         *  unit: seconds (1 sigma) */
                        static constexpr float_64 PULSE_LENGTH_SI = 4.0e-15;

                        /** beam waist: distance from the axis where the pulse␣
↪intensity (E^2)
                         *              decreases to its 1/e^2-th part,
                         *              at the focus position of the laser
                         *  unit: meter
                         */
                        static constexpr float_64 W0_X_SI = 4.246e-6; // waist in␣
↪x-direction
                        static constexpr float_64 W0_Z_SI = W0_X_SI; // waist in z-
↪direction

                        /** cell from top where the laser is initialized
                         *
                         * if `initPlaneY == 0` than the absorber are disabled.
                         * if `initPlaneY > absorbercells negative Y` the negative␣
↪absorber in y
                         * direction is enabled
                         *
                         * valid ranges:
                         *   - initPlaneY == 0
                         *   - absorber cells negative Y < initPlaneY < cells in y␣
↪direction of the top gpu
                         */
                        static constexpr uint32_t initPlaneY = 0;

                        /** laser phase shift (no shift: 0.0)
                         *
                         * sin(omega*time + laser_phase): starts with phase=0 at␣
↪center --> E-field=0 at center
                         *
                         * unit: rad, periodic in 2*pi
                         */
                        static constexpr float_X LASER_PHASE = 0.0;

                        /** Available polarization types
                         */
                        enum PolarisationType
                        {
                            LINEAR_X = 1u,
```

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```
                            LINEAR_Z = 2u,
                            CIRCULAR = 4u,
                        };
                        /** Polarization selection
                         */
                        static constexpr PolarisationType Polarisation = LINEAR_X;
                    };
                } // namespace defaults
            } // namespace polynom

            /** Wavepacket with a polynomial temporal intensity shape.
             *
             * Based on a wavepacket with Gaussian spatial envelope.
             *
             * @tparam T_Params class parameter to configure the polynomial laser␣
↪profile,
```

Plane Wave

template<typename **T_Params**>
struct PlaneWave : **public** *picongpu*::*fields*::*laserProfiles*::planeWave::Unitless<*T_Params*>

Plane wave laser profile.

Defines a plane wave with temporally Gaussian envelope.

Template Parameters

- T_Params: class parameter to configure the plane wave profile, see members of planeWave::defaults::PlaneWaveParam for required members

```
                    struct PlaneWaveParam
                    {
                        /** unit: meter */
                        static constexpr float_64 WAVE_LENGTH_SI = 0.8e-6;

                        /** Convert the normalized laser strength parameter a0 to␣
↪Volt per meter */
                        static constexpr float_64 UNITCONV_A0_to_Amplitude_SI = -2.
↪0 * PI / WAVE_LENGTH_SI
                            * ::picongpu::SI::ELECTRON_MASS_SI *␣
↪::picongpu::SI::SPEED_OF_LIGHT_SI
                            * ::picongpu::SI::SPEED_OF_LIGHT_SI /␣
↪::picongpu::SI::ELECTRON_CHARGE_SI;

                        /** unit: W / m^2 */
                        // calculate: _A0 = 8.549297e-6 * sqrt( Intensity[W/m^2] )␣
↪* wavelength[m] (linearly polarized)

                        /** unit: none */
                        static constexpr float_64 _A0 = 1.5;

                        /** unit: Volt / meter */
                        static constexpr float_64 AMPLITUDE_SI = _A0 * UNITCONV_A0_
↪to_Amplitude_SI;

                        /** unit: Volt / meter */
                        // static constexpr float_64 AMPLITUDE_SI = 1.738e13;

                        /** Stretch temporal profile by a constant plateau between␣
↪the up and downramp
```

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```
                         *  unit: seconds */
                        static constexpr float_64 LASER_NOFOCUS_CONSTANT_SI = 13.
↪34e-15;

                        /** Pulse length: sigma of std. gauss for intensity (E^2)
                         *  PULSE_LENGTH_SI = FWHM_of_Intensity   / [ 2*sqrt{ 2*␣
↪ln(2) } ]
                         *                                          [    2.
↪354820045     ]
                         *  Info:             FWHM_of_Intensity = FWHM_Illumination
                         *                      = what a experimentalist calls
↪"pulse duration"
                         *  unit: seconds (1 sigma) */
                        static constexpr float_64 PULSE_LENGTH_SI = 10.615e-15 / 4.
↪0;

                        /** cell from top where the laser is initialized
                         *
                         * if `initPlaneY == 0` than the absorber are disabled.
                         * if `initPlaneY > absorbercells negative Y` the negative␣
↪absorber in y
                         * direction is enabled
                         *
                         * valid ranges:
                         *   - initPlaneY == 0
                         *   - absorber cells negative Y < initPlaneY < cells in y␣
↪direction of the top gpu
                         */
                        static constexpr uint32_t initPlaneY = 0;

                        /** The laser pulse will be initialized half of PULSE_INIT␣
↪times of the PULSE_LENGTH before and
                         * after the plateau unit: none */
                        static constexpr float_64 RAMP_INIT = 20.6146;

                        /** laser phase shift (no shift: 0.0)
                         *
                         * sin(omega*time + laser_phase): starts with phase=0 at␣
↪center --> E-field=0 at center
                         *
                         * unit: rad, periodic in 2*pi
                         */
                        static constexpr float_X LASER_PHASE = 0.0;

                        /** Available polarization types
                         */
                        enum PolarisationType
                        {
                            LINEAR_X = 1u,
                            LINEAR_Z = 2u,
                            CIRCULAR = 4u,
                        };
                        /** Polarization selection
                         */
                        static constexpr PolarisationType Polarisation = LINEAR_X;
```

None

template<typename **T_Params**>
struct None : **public** *picongpu*::*fields*::*laserProfiles*::none::Unitless<*T_Params*>

Empty laser profile.

Does not define a laser profile but provides some hard-coded constants that are accessed directly in some places.

Template Parameters

- `T_Params`: class parameter to configure the "no laser" profile, see members of none::defaults::NoneParam for required members

incidentField.param

Load incident field parameters.

namespace picongpu

namespace fields

namespace incidentField

Unnamed Group

using XMin = None
Incident field source types along each boundary, these 6 types (or aliases) are required.

Each type has to be either Source<> or None.

using XMax = None

using YMin = None

using YMax = None

using ZMin = None

using ZMax = None

Typedefs

using MySource = Source<*FunctorIncidentE*, *FunctorIncidentB*>
Source of incident E and B fields.

Each source type combines functors for incident field E and B, which must be consistent to each other.

Variables

constexpr uint32_t picongpu::fields::incidentField::GAP_FROM_ABSORBER[3][2]=
Gap of the Huygence surface from absorber.

The gap is in cells, counted from the corrresponding boundary in the normal direction pointing inwards. It is similar to specifying absorber cells, just this layer is further inside.

class FunctorIncidentB
Functor to set values of incident B field.

Public Functions

PMACC_ALIGN (m_unitField, **const** float3_64)

HDINLINE **FunctorIncidentB** (**const** float3_64 *unitField*)
Create a functor.

Parameters
- `unitField`: conversion factor from SI to internal units, field_internal = field_SI / unitField

HDINLINE float3_X picongpu::fields::incidentField::FunctorIncidentB::opera
Calculate incident field B_inc(r, t) for a source.

Return incident field value in internal units
Parameters
- `totalCellIdx`: cell index in the total domain (including all moving window slides), note that it is fractional
- `currentStep`: current time step index, note that it is fractional

class FunctorIncidentE
Functor to set values of incident E field.

Public Functions

PMACC_ALIGN (m_unitField, **const** float3_64)

HDINLINE **FunctorIncidentE** (**const** float3_64 *unitField*)
Create a functor.

Parameters
- `unitField`: conversion factor from SI to internal units, field_internal = field_SI / unitField

HDINLINE float3_X picongpu::fields::incidentField::FunctorIncidentE::opera
Calculate incident field E_inc(r, t) for a source.

Return incident field value in internal units
Parameters
- `totalCellIdx`: cell index in the total domain (including all moving window slides), note that it is fractional
- `currentStep`: current time step index, note that it is fractional

pusher.param

Configure particle pushers.

Those pushers can then be selected by a particle species in species.param and speciesDefinition.param

namespace picongpu

struct particlePusherAccelerationParam
Subclassed by picongpu::particlePusherAcceleration::UnitlessParam

Public Static Attributes

constexpr float_64 **AMPLITUDEx_SI** = 0.0
Define strength of constant and homogeneous accelerating electric field in SI per dimension.

unit: Volt / meter

constexpr float_64 **AMPLITUDEy_SI** = -1.e11
The moving window propagation direction unit: Volt / meter (1e11 V/m = 1 GV/cm)

constexpr float_64 **AMPLITUDEz_SI** = 0.0
unit: Volt / meter

constexpr float_64 **ACCELERATION_TIME_SI** = 10000.0 * *picongpu*::*SI*::*DELTA_T_SI*
Acceleration duration unit: second.

namespace particlePusherAxel

Enums

enum TrajectoryInterpolationType
Values:

LINEAR = 1u

NONLINEAR = 2u

Variables

constexpr *TrajectoryInterpolationType* **TrajectoryInterpolation** = *LINEAR*

namespace particlePusherProbe

Typedefs

using ActualPusher = void
Also push the probe particles?

In many cases, probe particles are static throughout the simulation. This option allows to set an "actual" pusher that shall be used to also change the probe particle positions.

Examples:

- particles::pusher::Boris
- particles::pusher::[all others from above]
- void (no push)

density.param

Configure existing or define new normalized density profiles here.

During particle species creation in speciesInitialization.param, those profiles can be translated to spatial particle distributions.

namespace picongpu

namespace densityProfiles

Typedefs

using Gaussian = GaussianImpl<GaussianParam>

using Homogenous = HomogenousImpl

using LinearExponential = LinearExponentialImpl<LinearExponentialParam>

using GaussianCloud = GaussianCloudImpl<GaussianCloudParam>

using SphereFlanks = SphereFlanksImpl<SphereFlanksParam>

using FreeFormula = FreeFormulaImpl<*FreeFormulaFunctor*>

Functions

picongpu::densityProfiles::PMACC_STRUCT(GaussianParam, (PMACC_C_VALUE (float_X
Profile Formula: `const float_X exponent = abs((y - gasCenter_SI) / gasSigma_SI); const float_X density = exp(gasFactor * pow(exponent, gasPower));`

takes `gasCenterLeft_SI` for `y < gasCenterLeft_SI`, `gasCenterRight_SI` for `y > gasCenterRight_SI`, and `exponent = 0.0` for `gasCenterLeft_SI < y < gasCenterRight_SI`

picongpu::densityProfiles::PMACC_STRUCT(LinearExponentialParam, (PMACC_C_VALUE
parameter for `LinearExponential` profile

```
* Density Profile: /\
*                 /  ¯,_
*   linear       /      ¯,_    exponential
*   slope       /  |       ¯,_ slope
*                MAX
*
```

picongpu::densityProfiles::PMACC_STRUCT(GaussianCloudParam, (PMACC_C_VALUE (fl

picongpu::densityProfiles::PMACC_STRUCT(SphereFlanksParam, (PMACC_C_VALUE (uint
The profile consists out of the composition of 3 1D profiles with the scheme: exponential increasing flank, constant sphere, exponential decreasing flank.

```
*           ___
*  1D:  _,./   \./_   rho(r)
*
*  2D:  ..,x,..   density: . low
*       .,xxx,.            , middle
*       ..,x,..            x high (constant)
*
```

picongpu::densityProfiles::PMACC_STRUCT(FromOpenPMDParam, (PMACC_C_STRING (file
Density values taken from an openPMD file.

The density values must be a scalar dataset of type float_X, type mismatch would cause errors. This implementation would ignore all openPMD metadata but axisLabels. Each value in the dataset defines density in the cell with the corresponding total coordinate minus the given offset. When the functor is instantiated, it will load the part matching the current domain position. Density in points not present in the file would be set to the given default density. Dimensionality of the file indexing must match the simulation dimensionality. Density values are in BASE_DENSITY_SI units.

struct FreeFormulaFunctor

Public Functions

HDINLINE float_X picongpu::densityProfiles::FreeFormulaFunctor::operator()(c
This formula uses SI quantities only.

The profile will be multiplied by BASE_DENSITY_SI.

Return float_X density [normalized to 1.0]
Parameters

- `position_SI`: total offset including all slides [meter]

- `cellSize_SI`: cell sizes [meter]

namespace SI

Variables

constexpr float_64 **BASE_DENSITY_SI** = 1.e25
Base density in particles per m^3 in the density profiles.

This is often taken as reference maximum density in normalized profiles. Individual particle species can define a `densityRatio` flag relative to this value.

unit: ELEMENTS/m^3

speciesAttributes.param

This file defines available attributes that can be stored with each particle of a particle species.

Each attribute defined here needs to implement furthermore the traits

- Unit
- UnitDimension
- WeightingPower
- MacroWeighted in speciesAttributes.unitless for further information about these traits see therein.

namespace picongpu

Functions

alias(position)
relative (to cell origin) in-cell position of a particle

With this definition we do not define any type like float3_X, float3_64, ... This is only a name without a specialization.

value_identifier(uint64_t, particleId, IdProvider<*simDim*>::getNewId)
unique identifier for a particle

picongpu::value_identifier(floatD_X, position_pic, floatD_X::create (0.))
specialization for the relative in-cell position

picongpu::value_identifier(float3_X, momentum, float3_X::create (0.))
momentum at timestep t

picongpu::value_identifier(float3_X, momentumPrev1, float3_X::create (0._X))
momentum at (previous) timestep t-1

picongpu::value_identifier(float_X, weighting, 0. _X)
weighting of the macro particle

picongpu::value_identifier(int16_t, voronoiCellId, - 1)
Voronoi cell of the macro particle.

picongpu::value_identifier(float3_X, probeE, float3_X::create (0.))
interpolated electric field with respect to particle shape

Attribute can be added to any species.

picongpu::value_identifier(float3_X, probeB, float3_X::create (0.))
interpolated magnetic field with respect to particle shape

Attribute can be added to any species.

picongpu::value_identifier(bool, radiationMask, false)
masking a particle for radiation

The mask is used by the user defined filter `RadiationParticleFilter` in radiation.param to (de)select particles for the radiation calculation.

picongpu::value_identifier(bool, transitionRadiationMask, false)
masking a particle for transition radiation

The mask is used by the user defined filter `TransitionRadiationParticleFilter` in transitionRadiation.param to (de)select particles for the transition radiation calculation.

picongpu::value_identifier(float_X, boundElectrons, 0. _X)
number of electrons bound to the atom / ion

value type is float_X to avoid casts during the runtime

- float_X instead of integer types are reasonable because effective charge numbers are possible
- required for ion species if ionization is enabled
- setting it requires atomicNumbers to also be set

picongpu::value_identifier(flylite::Superconfig, superconfig, flylite::Superconfig:
atomic superconfiguration

atomic configuration of an ion for collisional-radiative modeling, see also flylite.param

value_identifier (DataSpace<*simDim*>, totalCellIdx, DataSpace<*simDim*>)
Total cell index of a particle.

The total cell index is a N-dimensional DataSpace given by a GPU's `globalDomain.offset` + `localDomain.offset` added to the N-dimensional cell index the particle belongs to on that GPU.

alias (shape)
alias for particle shape, see also species.param

alias (particlePusher)
alias for particle pusher, see alsospecies.param

alias (ionizers)
alias for particle ionizers, see also ionizer.param

alias (ionizationEnergies)
alias for ionization energy container, see also ionizationEnergies.param

alias (synchrotronPhotons)
alias for synchrotronPhotons, see also speciesDefinition.param

alias (bremsstrahlungIons)
alias for ion species used for bremsstrahlung

alias (bremsstrahlungPhotons)
alias for photon species used for bremsstrahlung

alias (interpolation)
alias for particle to field interpolation, see also species.param

alias (current)
alias for particle current solver, see also species.param

alias (atomicNumbers)
alias for particle flag: atomic numbers, see also ionizer.param

- only reasonable for atoms / ions / nuclei
- is required when boundElectrons is set

alias (effectiveNuclearCharge)
alias for particle flag: effective nuclear charge,

- see also ionizer.param
- only reasonable for atoms / ions / nuclei

alias (populationKinetics)
alias for particle population kinetics model (e.g.

FLYlite)

see also flylite.param

alias (massRatio)
alias for particle mass ratio

mass ratio between base particle, see also speciesConstants.param `SI::BASE_MASS_SI` and a user defined species

default value: 1.0 if unset

alias (chargeRatio)
alias for particle charge ratio

charge ratio between base particle, see also speciesConstants.param `SI::BASE_CHARGE_SI` and a user defined species

default value: 1.0 if unset

alias (densityRatio)
alias for particle density ratio

density ratio between default density, see also density.param `SI::BASE_DENSITY_SI` and a user defined species

default value: 1.0 if unset

alias (exchangeMemCfg)
alias to reserved bytes for each communication direction

This is an optional flag and overwrites the default species configuration in memory.param.

A memory config must be of the following form:

```
struct ExampleExchangeMemCfg
{
    static constexpr uint32_t BYTES_EXCHANGE_X = 5 * 1024 * 1024;
    static constexpr uint32_t BYTES_EXCHANGE_Y = 5 * 1024 * 1024;
    static constexpr uint32_t BYTES_EXCHANGE_Z = 5 * 1024 * 1024;
    static constexpr uint32_t BYTES_CORNER = 16 * 1024;
    static constexpr uint32_t BYTES_EDGES = 16 * 1024;
    using REF_LOCAL_DOM_SIZE = mCT::Int<0, 0, 0>;
    const std::array<float_X, 3> DIR_SCALING_FACTOR = {{0.0, 0.0, 0.0}};
};
```

alias (boundaryCondition)
alias to specify the internal pmacc boundary treatment for particles

It controls the internal behavior and intented for special cases only. To set physical boundary conditions for a species, instead use <species>_boundary command-line option.

The default behavior if this alias is not given to a species is to do nothing. The existing boundary implementations already take care of the particles leaving the global simulation volume.

The following species attributes are defined by PMacc and always stored with a particle:

namespace pmacc

Functions

pmacc::value_identifier(lcellId_t, localCellIdx, 0)
cell of a particle inside a supercell

Value is a linear cell index inside the supercell

pmacc::value_identifier(uint8_t, multiMask, 0)
state of a particle

Particle might be valid or invalid in a particle frame. Valid particles can further be marked as candidates to leave a supercell. Possible multiMask values are:

- 0 (zero): no particle (invalid)
- 1: particle (valid)
- 2 to 27: (valid) particle that is about to leave its supercell but is still stored in the current particle frame. Directions to leave the supercell are defined as follows. An ExchangeType = value - 1 (e.g. 27 - 1 = 26) means particle leaves supercell in the direction of FRONT(value=18) && TOP(value=6) && LEFT(value=2) which defines a diagonal movement over a supercell corner (18+6+2=26).

speciesConstants.param

Constants and thresholds for particle species.

Defines the reference mass and reference charge to express species with (default: electrons with negative charge).

namespace picongpu

Variables

constexpr float_X picongpu::GAMMA_THRESH = 1.005_X
Threshold between relativistic and non-relativistic regime.

Threshold used for calculations that want to separate between high-precision formulas for relativistic and non-relativistic use-cases, e.g. energy-binning algorithms.

constexpr float_X picongpu::GAMMA_INV_SQUARE_RAD_THRESH = 0.18_X
Threshold in radiation plugin between relativistic and non-relativistic regime.

This limit is used to decide between a pure 1-sqrt(1-x) calculation and a 5th order Taylor approximation of 1-sqrt(1-x) to avoid halving of significant digits due to the sqrt() evaluation at x = 1/gamma^2 near 0.0. With 0.18 the relative error between Taylor approximation and real value will be below 0.001% = 1e-5 * for x=1/gamma^2 < 0.18

namespace SI

Variables

constexpr float_64 **BASE_MASS_SI** = *ELECTRON_MASS_SI*
base particle mass

reference for massRatio in speciesDefinition.param

unit: kg

constexpr float_64 **BASE_CHARGE_SI** = *ELECTRON_CHARGE_SI*
base particle charge

reference for chargeRatio in speciesDefinition.param

unit: C

species.param

Particle shape, field to particle interpolation, current solver, and particle pusher can be declared here for usage in `speciesDefinition.param`.

See **MODELS / Hierarchy of Charge Assignment Schemes** in the online documentation for information on particle shapes.

Attention The higher order shape names are redefined with release 0.6.0 in order to provide a consistent naming:

- PQS is the name of the 3rd order assignment function (instead of PCS)
- PCS is the name of the 4th order assignment function (instead of P4S)
- P4S does not exist anymore

namespace picongpu

Typedefs

using UsedParticleShape = *particles*::shapes::TSC
select macroparticle shape

WARNING the shape names are redefined and diverge from PIConGPU versions before 0.6.0.

- particles::shapes::CIC : Assignment function is a piecewise linear spline
- particles::shapes::TSC : Assignment function is a piecewise quadratic spline
- particles::shapes::PQS : Assignment function is a piecewise cubic spline
- particles::shapes::PCS : Assignment function is a piecewise quartic spline

using UsedField2Particle = FieldToParticleInterpolation<*UsedParticleShape*, AssignedTrilinearInterpolation>
select interpolation method to be used for interpolation of grid-based field values to particle positions

using UsedParticleCurrentSolver = currentSolver::Esirkepov<*UsedParticleShape*>
select current solver method

- currentSolver::Esirkepov< SHAPE, STRATEGY > : particle shapes - CIC, TSC, PQS, PCS (1st to 4th order)
- currentSolver::VillaBune< SHAPE, STRATEGY > : particle shapes - CIC (1st order) only
- currentSolver::EmZ< SHAPE, STRATEGY > : particle shapes - CIC, TSC, PQS, PCS (1st to 4th order)

For development purposes:

- currentSolver::EsirkepovNative< SHAPE, STRATEGY > : generic version of currentSolverEsirkepov without optimization (~4x slower and needs more shared memory)

STRATEGY (optional):

- currentSolver::strategy::StridedCachedSupercells
- currentSolver::strategy::StridedCachedSupercellsScaled<N> with N >= 1
- currentSolver::strategy::CachedSupercells
- currentSolver::strategy::CachedSupercellsScaled<N> with N >= 1
- currentSolver::strategy::NonCachedSupercells
- currentSolver::strategy::NonCachedSupercellsScaled<N> with N >= 1

using UsedParticlePusher = *particles*::pusher::Boris
particle pusher configuration

Defining a pusher is optional for particles

- particles::pusher::HigueraCary : Higuera & Cary's relativistic pusher preserving both volume and ExB velocity
- particles::pusher::Vay : Vay's relativistic pusher preserving ExB velocity
- particles::pusher::Boris : Boris' relativistic pusher preserving volume
- particles::pusher::ReducedLandauLifshitz : 4th order RungeKutta pusher with classical radiation reaction
- particles::pusher::Composite : composite of two given pushers, switches between using one (or none) of those

For diagnostics & modeling: ————————————————

- particles::pusher::Acceleration : Accelerate particles by applying a constant electric field
- particles::pusher::Free : free propagation, ignore fields (= free stream model)
- particles::pusher::Photon : propagate with c in direction of normalized mom.
- particles::pusher::Probe : Probe particles that interpolate E & B For development purposes: ————————————————
- particles::pusher::Axel : a pusher developed at HZDR during 2011 (testing)

Current solver details.

speciesDefinition.param

Define particle species.

This file collects all previous declarations of base (reference) quantities and configured solvers for species and defines particle species. This includes "attributes" (lvalues to store with each species) and "flags" (rvalues & aliases for solvers to perform with the species for each timestep and ratios to base quantities). With those information, a `Particles` class is defined for each species and then collected in the list `VectorAllSpecies`.

namespace picongpu

Typedefs

using DefaultParticleAttributes = MakeSeq_t<position<position_pic>, momentum, weighting>
describe attributes of a particle

using ParticleFlagsPhotons = MakeSeq_t<particlePusher<*particles*::pusher::Photon>, shape<*UsedParticleShape*>

using PIC_Photons = Particles<PMACC_CSTRING("ph"), *ParticleFlagsPhotons*, *DefaultParticleAttributes*>

using ParticleFlagsElectrons = MakeSeq_t<particlePusher<*UsedParticlePusher*>, shape<*UsedParticleShape*>, i

using PIC_Electrons = Particles<PMACC_CSTRING("e"), *ParticleFlagsElectrons*, *DefaultParticleAttributes*>

using ParticleFlagsIons = MakeSeq_t<particlePusher<*UsedParticlePusher*>, shape<*UsedParticleShape*>, interpol

using PIC_Ions = Particles<PMACC_CSTRING("i"), *ParticleFlagsIons*, *DefaultParticleAttributes*>

using VectorAllSpecies = MakeSeq_t<*PIC_Electrons*, *PIC_Ions*>
All known particle species of the simulation.

List all defined particle species from above in this list to make them available to the PIC algorithm.

Functions

picongpu::value_identifier(float_X, MassRatioPhotons, 0. 0)

picongpu::value_identifier(float_X, ChargeRatioPhotons, 0. 0)

picongpu::value_identifier(float_X, MassRatioElectrons, 1. 0)

picongpu::value_identifier(float_X, ChargeRatioElectrons, 1. 0)

picongpu::value_identifier(float_X, MassRatioIons, 1836. 152672)

picongpu::value_identifier(float_X, ChargeRatioIons, -1. 0)

picongpu::value_identifier(float_X, DensityRatioIons, 1. 0)

particle.param

Configurations for particle manipulators.

Set up and declare functors that can be used in speciesInitalization.param for particle species initialization and manipulation, such as temperature distributions, drifts, pre-ionization and in-cell position.

namespace picongpu

namespace particles

Variables

constexpr float_X **MIN_WEIGHTING** = 10.0
a particle with a weighting below MIN_WEIGHTING will not be created / will be deleted

unit: none

constexpr uint32_t **TYPICAL_PARTICLES_PER_CELL** = 2u
Number of maximum particles per cell during density profile evaluation.

Determines the weighting of a macro particle and with it, the number of particles "sampling" dynamics in phase space.

namespace manipulators

Typedefs

using AssignXDrift = unary::*Drift*<*DriftParam*, *pmacc*::math::operation::Assign>
definition of manipulator that assigns a drift in X

using AddTemperature = unary::*Temperature*<*TemperatureParam*>

using DoubleWeighting = generic::*Free*<*DoubleWeightingFunctor*>
definition of a free particle manipulator: double weighting

using RandomEnabledRadiation = generic::*FreeRng*<*RandomEnabledRadiationFunctor*, *pmacc*::rando

using RandomPosition = unary::*RandomPosition*
changes the in-cell position of each particle of a species

Functions

picongpu::particles::manipulators::CONST_VECTOR(float_X, 3, DriftParam_direc
Parameter for DriftParam.

struct DoubleWeightingFunctor
Unary particle manipulator: double each weighting.

Public Functions

template<typename T_Particle>DINLINE void picongpu::particles::manipulato

struct DriftParam
Parameter for a particle drift assignment.

Public Members

const DriftParam_direction_t **direction**

Public Static Attributes

constexpr float_64 **gamma** = 1.0

struct RandomEnabledRadiationFunctor

Public Functions

template<typename T_Rng, typename T_Particle>DINLINE void picongpu::parti

struct TemperatureParam
Parameter for a temperature assignment.

Public Static Attributes

constexpr float_64 **temperature** = 0.0

namespace startPosition

Typedefs

using Random = RandomImpl<*RandomParameter*>
definition of random particle start

using Quiet = QuietImpl<*QuietParam*>
definition of quiet particle start

using OnePosition = OnePositionImpl<*OnePositionParameter*>
definition of one specific position for particle start

Functions

picongpu::particles::startPosition::CONST_VECTOR(float_X, 3, InCellOffset, C
sit directly in lower corner of the cell

struct OnePositionParameter

Public Members

const InCellOffset_t **inCellOffset**

Public Static Attributes

constexpr uint32_t **numParticlesPerCell** = *TYPICAL_PARTICLES_PER_CELL*
Count of particles per cell at initial state.

unit: none

struct QuietParam

Public Types

using numParticlesPerDimension = mCT::shrinkTo<mCT::Int<1, *TYPICAL_PARTICLES_PER_C*
Count of particles per cell per direction at initial state.

unit: none

struct RandomParameter

Public Static Attributes

constexpr uint32_t **numParticlesPerCell** = *TYPICAL_PARTICLES_PER_CELL*
Count of particles per cell at initial state.

unit: none

More details on the order of initialization of particles inside a particle species *can be found here*.

List of all pre-defined particle manipulators.

unit.param

In this file we define typical scales for normalization of physical quantities aka "units".

Usually, a user would not change this file but might use the defined constants in other input files.

namespace picongpu

Variables

constexpr float_64 **UNIT_TIME** = *SI*::*DELTA_T_SI*
Unit of time.

constexpr float_64 **UNIT_LENGTH** = *UNIT_TIME* * *UNIT_SPEED*
Unit of length.

constexpr float_64 **UNIT_MASS** = *SI*::*BASE_MASS_SI* * double(*particles*::*TYPICAL_NUM_PARTICLES_PER_MACRO*
Unit of mass.

constexpr float_64 **UNIT_CHARGE** = -1.0 * *SI*::*BASE_CHARGE_SI* * double(*particles*::*TYPICAL_NUM_PARTICLES_P*
Unit of charge.

constexpr float_64 **UNIT_ENERGY** = (*UNIT_MASS* * *UNIT_LENGTH* * *UNIT_LENGTH* / (*UNIT_TIME* * *UNIT_TIME*
Unit of energy.

constexpr float_64 **UNIT_EFIELD** = 1.0 / (*UNIT_TIME* * *UNIT_TIME* / *UNIT_MASS* / *UNIT_LENGTH* * *UNIT_CHAR*
Unit of EField: V/m.

constexpr float_64 **UNIT_BFIELD** = (*UNIT_MASS* / (*UNIT_TIME* * *UNIT_CHARGE*))

namespace particles

Variables

constexpr float_X **TYPICAL_NUM_PARTICLES_PER_MACROPARTICLE** = float_64(*SI*::*BASE_DENSITY_SI* *
Number of particles per makro particle (= macro particle weighting) unit: none.

particleFilters.param

A common task in both modeling and in situ processing (output) is the selection of particles of a particle species by attributes.

Users can define such selections as particle filters in this file.

Particle filters are simple mappings assigning each particle of a species either `true` or `false` (ignore / filter out).

All active filters need to be listed in `AllParticleFilters`. They are then combined with `VectorAllSpecies` at compile-time, e.g. for plugins.

namespace picongpu

namespace particles

namespace filter

Typedefs

using AllParticleFilters = MakeSeq_t<*All*>
Plugins: collection of all available particle filters.

Create a list of all filters here that you want to use in plugins.

Note: filter *All* is defined in picongpu/particles/filter/filter.def

List of all pre-defined particle filters.

speciesInitialization.param

Initialize particles inside particle species.

This is the final step in setting up particles (defined in `speciesDefinition.param`) via density profiles (defined in `density.param`). One can then further derive particles from one species to another and manipulate attributes with "manipulators" and "filters" (defined in `particle.param` and `particleFilters.param`).

namespace picongpu

namespace particles

Typedefs

using InitPipeline = bmpl::vector<>
InitPipeline defines in which order species are initialized.

the functors are called in order (from first to last functor). The functors must be default-constructible and take the current time iteration as the only parameter.

List of all initialization methods for particle species.

Particles

Particles are defined in modular steps. First, species need to be generally defined in *speciesDefinition.param*. Second, species are initialized with particles in *speciesInitialization.param*.

The following operations can be applied in the `picongpu::particles::InitPipeline` of the latter:

Initialization

CreateDensity

template<typename **T_DensityFunctor**, typename **T_PositionFunctor**, typename **T_SpeciesType** = bmpl::_1>
struct CreateDensity

Sample macroparticles according to the given spatial density profile.

Create macroparticles inside a species.

This function only concerns the number of macroparticles, positions, and weighting. So it basically performs sampling in the coordinate space, while not initializing other attributes. When needed, those should be set (for then-existing macroparticles) by subsequently calling *Manipulate*.

User input to this functor is two-fold. T_DensityFunctor represents spatial density of real particles, normalized according to our requirements. It describes the physical setup being simulated and only deals with real, not macro-, particles. T_PositionFunctor is more of a PIC simulation parameter. It defines how real particles in each cell will be represented with macroparticles. This concerns the count, weighting, and in-cell positions of the created macroparticles.

The sampling process operates independently for each cell, as follows:

- Evaluate the amount of real particles in the cell, Nr, using T_DensityFunctor.
- If Nr > 0, decide how to represent it with macroparticles using T_PositionFunctor:
  - (For simplicity we describe how all currently used functors operate, see below for customization)
  - Try to have exactly T_PositionFunctor::numParticlesPerCell macroparticles with same weighting w = Nr / T_PositionFunctor::numParticlesPerCell.
  - If such w < MIN_WEIGHTING, instead use fewer macroparticles and higher weighting.
  - In any case the combined weighting of all new macroparticles will match Nr.
- Create the selected number of macroparticles with selected weighting.
- Set in-cell positions according to T_PositionFunctor.

In principle, one could override the logic inside the (If Nr > 0) block by implementing a custom functor. Then one could have an arbitrary number of macroparticles and weight distribution between them. The only requirement is that together it matches Nr. However, the description above holds for all preset position functors provided by PIConGPU. Note that in this scheme almost all non-vacuum cells will start with the same number of macroparticles. Having a higher density in a cell would mean larger weighting, but not more macroparticles.

Note *FillAllGaps* is automatically called after creation.

Template Parameters

- `T_DensityFunctor`: unary lambda functor with profile description, see density.param, example: picongpu::particles::densityProfiles::Homogenous
- `T_PositionFunctor`: unary lambda functor with position description and number of macroparticles per cell, see particle.param, examples: picongpu::particles::startPosition::Quiet, picongpu::particles::startPosition::Random

- `T_SpeciesType`: type or name as boost::mpl::string of the used species, see speciesDefinition.param

Derive

template<typename **`T_SrcSpeciesType`**, typename **`T_DestSpeciesType`** = bmpl::_1, typename **`T_Filter`** = *filter*::*All*>
`struct Derive` : **`public`** *picongpu*::*particles*::*ManipulateDerive*<*manipulators*::generic::None, *T_SrcSpeciesType*, *T_DestSp*

Generate particles in a species by deriving from another species' particles.

Create particles in `T_DestSpeciesType` by deriving (copying) all particles and their matching attributes (except `particleId`) from `T_SrcSpeciesType`.

Note *FillAllGaps* is called on on `T_DestSpeciesType` after the derivation is finished.

Template Parameters

- `T_SrcSpeciesType`: type or name as boost::mpl::string of the source species
- `T_DestSpeciesType`: type or name as boost::mpl::string of the destination species
- `T_Filter`: picongpu::particles::filter, particle filter type to select source particles to derive

Manipulate

template<typename **`T_Manipulator`**, typename **`T_Species`** = bmpl::_1, typename **`T_Filter`** = *filter*::*All*, typename **`T_Are`**
`struct Manipulate` : **`public`** *pmacc*::particles::algorithm::CallForEach<*pmacc*::particles::meta::FindByNameOrType<*Vecto*

Run a user defined manipulation for each particle of a species in an area.

Allows to manipulate attributes of existing particles in a species with arbitrary unary functors ("manipulators").

Provides two versions of operator() to either operate on T_Area or a custom area,

See pmacc::particles::algorithm::CallForEach.

Warning Does NOT call *FillAllGaps* after manipulation! If the manipulation deactivates particles or creates "gaps" in any other way, *FillAllGaps* needs to be called for the `T_Species` manually in the next step!

See picongpu::particles::manipulators

Template Parameters

- `T_Manipulator`: unary lambda functor accepting one particle species,

Template Parameters

- `T_Species`: type or name as boost::mpl::string of the used species
- `T_Filter`: picongpu::particles::filter, particle filter type to select particles in `T_Species` to manipulate
- `T_Area`: area to process particles in operator()(currentStep), wrapped into std::integral_constant for boost::mpl::apply to work; does not affect operator()(currentStep, areaMapperFactory)

ManipulateDerive

template<typename **`T_Manipulator`**, typename **`T_SrcSpeciesType`**, typename **`T_DestSpeciesType`** = bmpl::_1, typena
`struct ManipulateDerive`

Generate particles in a species by deriving and manipulating from another species' particles.

Create particles in `T_DestSpeciesType` by deriving (copying) all particles and their matching attributes (except `particleId`) from `T_SrcSpeciesType`. During the derivation, the particle attributes in can be manipulated with `T_ManipulateFunctor`.

Note *FillAllGaps* is called on on T_DestSpeciesType after the derivation is finished. If the derivation also manipulates the T_SrcSpeciesType, e.g. in order to deactivate some particles for a move, *FillAllGaps* needs to be called for the T_SrcSpeciesType manually in the next step!

See picongpu::particles::manipulators

Template Parameters

- `T_Manipulator`: a pseudo-binary functor accepting two particle species: destination and source,

Template Parameters

- `T_SrcSpeciesType`: type or name as boost::mpl::string of the source species
- `T_DestSpeciesType`: type or name as boost::mpl::string of the destination species
- `T_SrcFilter`: picongpu::particles::filter, particle filter type to select particles in T_SrcSpeciesType to derive into T_DestSpeciesType

FillAllGaps

template<typename **`T_SpeciesType`** = bmpl::_1>
`struct FillAllGaps`

Generate a valid, contiguous list of particle frames.

Some operations, such as deactivating or adding particles to a particle species can generate "gaps" in our internal particle storage, a list of frames.

This operation copies all particles from the end of the frame list to "gaps" in the beginning of the frame list. After execution, the requirement that all particle frames must be filled contiguously with valid particles and that all frames but the last are full is fulfilled.

Template Parameters

- `T_SpeciesType`: type or name as boost::mpl::string of the particle species to fill gaps in memory

Manipulation Functors

Some of the particle operations above can take the following functors as arguments to manipulate attributes of particle species. A particle filter (see following section) is used to only manipulated selected particles of a species with a functor.

Free

template<typename **`T_Functor`**>
`struct Free` : **`protected`** *picongpu*::*particles*::functor::User<*T_Functor*>

call simple free user defined manipulators

example for `particle.param`: set in cell position to zero

```
struct FunctorInCellPositionZero
{
    template< typename T_Particle >
    HDINLINE void operator()( T_Particle & particle )
```

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```
    {
        particle[ position_ ] = floatD_X::create( 0.0 );
    }
    static constexpr char const * name = "inCellPositionZero";
};

using InCellPositionZero = generic::Free<
   FunctorInCellPositionZero
>;
```

Template Parameters

- `T_Functor`: user defined manipulators **optional**: can implement **one** host side constructor `T_Functor()` or `T_Functor(uint32_t currentTimeStep)`

FreeRng

template<typename **`T_Functor`**, typename **`T_Distribution`**>
`struct FreeRng` : **`protected`** *picongpu*::*particles*::functor::User<*T_Functor*>, **`private`** *picongpu*::*particles*::functor::misc

call simple free user defined functor and provide a random number generator

example for `particle.param`: add

```
#include <pmacc/random/distributions/Uniform.hpp>

struct FunctorRandomX
{
    template< typename T_Rng, typename T_Particle >
    HDINLINE void operator()( T_Rng& rng, T_Particle& particle )
    {
        particle[ position_ ].x() = rng();
    }
    static constexpr char const * name = "randomXPos";
};

using RandomXPos = generic::FreeRng<
   FunctorRandomX,
   pmacc::random::distributions::Uniform< float_X >
>;
```

Template Parameters

- `T_Functor`: user defined unary functor
- `T_Distribution`: pmacc::random::distributions, random number distribution

and to `InitPipeline` in `speciesInitialization.param`:

```
Manipulate< manipulators::RandomXPos, SPECIES_NAME >
```

FreeTotalCellOffset

template<typename **`T_Functor`**>
`struct FreeTotalCellOffset` : **`protected`** *picongpu*::*particles*::functor::User<*T_Functor*>, **`private`** *picongpu*::*parti*

call simple free user defined manipulators and provide the cell information

The functor passes the cell offset of the particle relative to the total domain origin into the functor.

example for `particle.param`: set a user-defined species attribute y0 (type: uint32_t) to the current total y-cell index

```
struct FunctorSaveYcell
{
    template< typename T_Particle >
    HDINLINE void operator()(
       DataSpace< simDim > const & particleOffsetToTotalOrigin,
       T_Particle & particle
    )
    {
        particle[ y0_ ] = particleOffsetToTotalOrigin.y();
    }
    static constexpr char const * name = "saveYcell";
};

using SaveYcell = unary::FreeTotalCellOffset<
   FunctorSaveYcell
>;
```

Template Parameters

- `T_Functor`: user defined unary functor

CopyAttribute

using *picongpu*::*particles*::*manipulators*::unary::**CopyAttribute** = generic::*Free*<acc::CopyAttribute<T_
copy a particle source attribute to a destination attribute

This is an unary functor and operates on one particle.

Template Parameters

- `T_DestAttribute`: type of the destination attribute e.g. `momentumPrev1`
- `T_SrcAttribute`: type of the source attribute e.g. `momentum`

Drift

using *picongpu*::*particles*::*manipulators*::unary::**Drift** = generic::*Free*<acc::Drift<T_ParamClass, T_Value
change particle's momentum based on speed

allow to manipulate a speed to a particle

Template Parameters

- `T_ParamClass`: param::DriftCfg, configuration parameter
- `T_ValueFunctor`: pmacc::math::operation::*, binary functor type to manipulate the momentum attribute

RandomPosition

using *picongpu*::*particles*::*manipulators*::unary::**RandomPosition** = generic::*FreeRng*<acc::RandomPos
Change the in cell position.

This functor changes the in-cell position of a particle. The new in-cell position is uniformly distributed position between [0.0;1.0).

example: add

```
particles::Manipulate<RandomPosition,SPECIES_NAME>
```

to `InitPipeline` in `speciesInitialization.param`

Temperature

using *picongpu*::*particles*::*manipulators*::unary::**Temperature** = generic::*FreeRng*<acc::Temperature<T_
Modify particle momentum based on temperature.

note: initial electron temperature should generally be chosen so that the resulting Debye length is resolved by the grid.

Template Parameters

- `T_ParamClass`: param::TemperatureCfg, configuration parameter
- `T_ValueFunctor`: pmacc::math::operation::*, binary functor type to add a new momentum to an old one

Assign

using *picongpu*::*particles*::*manipulators*::binary::**Assign** = generic::*Free*<acc::Assign>
assign attributes of one particle to another

Can be used as binary and higher order operator but only the first two particles are used for the assign operation.

Assign all matching attributes of a source particle to the destination particle. Attributes that only exist in the destination species are initialized with the default value. Attributes that only exists in the source particle will be ignored.

DensityWeighting

using *picongpu*::*particles*::*manipulators*::binary::**DensityWeighting** = generic::*Free*<acc::DensityWei
Re-scale the weighting of a cloned species by densityRatio.

When deriving species from each other, the new species "inherits" the macro-particle weighting of the first one. This functor can be used to manipulate the weighting of the new species' macro particles to satisfy the input densityRatio of it.

note: needs the densityRatio flag on both species, used by the GetDensityRatio trait.

ProtonTimesWeighting

using *picongpu*::*particles*::*manipulators*::binary::**ProtonTimesWeighting** = generic::*Free*<acc::Proton
Re-scale the weighting of a cloned species by numberOfProtons.

When deriving species from each other, the new species "inherits" the macro-particle weighting of the first one. This functor can be used to manipulate the weighting of the new species' macro particles to be a multiplied by the number of protons of the initial species.

As an example, this is useful when initializing a quasi-neutral, pre-ionized plasma of ions and electrons. Electrons can be created from ions via deriving and increasing their weight to avoid simulating multiple macro electrons per macro ion (with Z>1).

note: needs the atomicNumbers flag on the initial species, used by the GetAtomicNumbers trait.

Manipulation Filters

Most of the particle functors shall operate on all valid particles, where `filter::All` is the default assumption. One can limit the domain or subset of particles with filters such as the ones below (or define new ones).

All

struct All

RelativeGlobalDomainPosition

template<typename **T_Params**>
struct RelativeGlobalDomainPosition
filter particle dependent on the global position

Check if a particle is within a relative area in one direction of the global domain.

Template Parameters

- `T_Params`: picongpu::particles::filter::param::RelativeGlobalDomainPosition, parameter to configure the functor

Free

template<typename **T_Functor**>
struct Free : **protected** *picongpu*::*particles*::functor::User<*T_Functor*>
call simple free user defined filter

example for `particleFilters.param`: each particle with in-cell position greater than 0.5

```
struct FunctorEachParticleAboveMiddleOfTheCell
{
    template< typename T_Particle >
    HDINLINE bool operator()( T_Particle const & particle )
    {
        bool result = false;
        if( particle[ position_ ].y() >= float_X( 0.5 ) )
            result = true;
        return result;
    }
    static constexpr char const * name = "eachParticleAboveMiddleOfTheCell";
};

using EachParticleAboveMiddleOfTheCell = generic::Free<
   FunctorEachParticleAboveMiddleOfTheCell
>;
```

Template Parameters

- `T_Functor`: user defined filter **optional**: can implement **one** host side constructor `T_Functor()` or `T_Functor(uint32_t currentTimeStep)`

FreeRng

template<typename **T_Functor**, typename **T_Distribution**>

struct FreeRng : **protected** *picongpu*::*particles*::functor::User<*T_Functor*>, **private** *picongpu*::*particles*::functor::misc
call simple free user defined functor and provide a random number generator

example for `particleFilters.param`: get every second particle (random sample of 50%)

```
struct FunctorEachSecondParticle
{
    template< typename T_Rng, typename T_Particle >
    HDINLINE bool operator()(
        T_Rng & rng,
        T_Particle const & particle
    )
    {
        bool result = false;
        if( rng() >= float_X( 0.5 ) )
            result = true;
        return result;
    }
    static constexpr char const * name = "eachSecondParticle";
};

using EachSecondParticle = generic::FreeRng<
   FunctorEachSecondParticle,
   pmacc::random::distributions::Uniform< float_X >
>;
```

Template Parameters

- `T_Functor`: user defined unary functor
- `T_Distribution`: pmacc::random::distributions, random number distribution

FreeTotalCellOffset

template<typename **T_Functor**>
struct FreeTotalCellOffset : **protected** *picongpu*::*particles*::functor::User<*T_Functor*>, **private** *picongpu*::*partic*
call simple free user defined functor and provide the cell information

The functor passes the cell offset of the particle relative to the total domain origin into the functor.

example for `particleFilters.param`: each particle with a cell offset of 5 in X direction

```
struct FunctorEachParticleInXCell5
{
    template< typename T_Particle >
    HDINLINE bool operator()(
        DataSpace< simDim > const & particleOffsetToTotalOrigin,
        T_Particle const & particle
    )
    {
        bool result = false;
        if( particleOffsetToTotalOrigin.x() == 5 )
            result = true;
        return result;
    }
    static constexpr char const * name = "eachParticleInXCell5";
};

using EachParticleInXCell5 = generic::FreeTotalCellOffset<
   FunctorEachParticleInXCell5
>;
```

Template Parameters

- `T_Functor`: user defined unary functor

Memory

memory.param

Define low-level memory settings for compute devices.

Settings for memory layout for supercells and particle frame-lists, data exchanges in multi-device domain-decomposition and reserved fields for temporarily derived quantities are defined here.

namespace picongpu

Typedefs

using SuperCellSize = **typename** mCT::shrinkTo<mCT::Int<8, 8, 4>, *simDim*>::type
size of a superCell

volume of a superCell must be <= 1024

using MappingDesc = MappingDescription<*simDim*, *SuperCellSize*>
define mapper which is used for kernel call mappings

using GuardSize = **typename** mCT::shrinkTo<mCT::Int<1, 1, 1>, *simDim*>::type
define the size of the core, border and guard area

PIConGPU uses spatial domain-decomposition for parallelization over multiple devices with non-shared memory architecture. The global spatial domain is organized per device in three sections: the GUARD area contains copies of neighboring devices (also known as "halo"/"ghost"). The BORDER area is the outermost layer of cells of a device, equally to what neighboring devices see as GUARD area. The CORE area is the innermost area of a device. In union with the BORDER area it defines the "active" spatial domain on a device.

GuardSize is defined in units of SuperCellSize per dimension.

Variables

constexpr size_t **reservedGpuMemorySize** = 350 * 1024 * 1024

constexpr uint32_t **fieldTmpNumSlots** = 1
number of scalar fields that are reserved as temporary fields

constexpr bool **fieldTmpSupportGatherCommunication** = true
can *FieldTmp* gather neighbor information

If `true` it is possible to call the method `asyncCommunicationGather()` to copy data from the border of neighboring GPU into the local guard. This is also known as building up a "ghost" or "halo" region in domain decomposition and only necessary for specific algorithms that extend the basic PIC cycle, e.g. with dependence on derived density or energy fields.

struct DefaultExchangeMemCfg
bytes reserved for species exchange buffer

This is the default configuration for species exchanges buffer sizes. The default exchange buffer sizes can be changed per species by adding the alias exchangeMemCfg with similar members like in DefaultExchangeMemCfg to its flag list.

Public Types

using REF_LOCAL_DOM_SIZE = mCT::Int<0, 0, 0>
Reference local domain size.

The size of the local domain for which the exchange sizes `BYTES_*` are configured for. The required size of each exchange will be calculated at runtime based on the local domain size and the reference size. The exchange size will be scaled only up and not down. Zero means that there is no reference domain size, exchanges will not be scaled.

Public Members

const std::array<float_X, 3> picongpu::DefaultExchangeMemCfg::DIR_SCALING_FACTO
Scaling rate per direction.

1.0 means it scales linear with the ratio between the local domain size at runtime and the reference local domain size.

Public Static Attributes

constexpr uint32_t **BYTES_EXCHANGE_X** = 1 * 1024 * 1024

constexpr uint32_t **BYTES_EXCHANGE_Y** = 3 * 1024 * 1024

constexpr uint32_t **BYTES_EXCHANGE_Z** = 1 * 1024 * 1024

constexpr uint32_t **BYTES_EDGES** = 32 * 1024

constexpr uint32_t **BYTES_CORNER** = 8 * 1024

precision.param

Define the precision of typically used floating point types in the simulation.

PIConGPU normalizes input automatically, allowing to use single-precision by default for the core algorithms. Note that implementations of various algorithms (usually plugins or non-core components) might still decide to hard-code a different (mixed) precision for some critical operations.

mallocMC.param

Fine-tuning of the particle heap for GPUs: When running on GPUs, we use a high-performance parallel "new" allocator (mallocMC) which can be parametrized here.

namespace picongpu

Typedefs

using DeviceHeap = mallocMC::Allocator<cupla::Acc, mallocMC::CreationPolicies::Scatter<*DeviceHeapConfig*>, mal
Define a new allocator.

This is an allocator resembling the behaviour of the ScatterAlloc algorithm.

struct DeviceHeapConfig
configure the CreationPolicy "Scatter"

Public Static Attributes

constexpr uint32_t **pagesize** = 2u * 1024u * 1024u
2MiB page can hold around 256 particle frames

constexpr uint32_t **accessblocksize** = 2u * 1024u * 1024u * 1024u
accessblocksize, regionsize and wastefactor are not conclusively investigated and might be performance sensitive for multiple particle species with heavily varying attributes (frame sizes)

constexpr uint32_t **regionsize** = 16u

constexpr uint32_t **wastefactor** = 2u

constexpr bool **resetfreedpages** = true
resetfreedpages is used to minimize memory fragmentation with varying frame sizes

PIC Extensions

fieldBackground.param

Load external background fields.

namespace picongpu

class FieldBackgroundB

Public Functions

PMACC_ALIGN(m_unitField, **const** float3_64)

HDINLINE **FieldBackgroundB**(**const** float3_64 *unitField*)

HDINLINE float3_X picongpu::FieldBackgroundB::operator()(const DataSpace < sim
Specify your background field B(r,t) here.

Parameters

- `cellIdx`: The total cell id counted from the start at t=0
- `currentStep`: The current time step

Public Static Attributes

constexpr bool **InfluenceParticlePusher** = false

class FieldBackgroundE

Public Functions

PMACC_ALIGN(m_unitField, **const** float3_64)

HDINLINE **FieldBackgroundE**(**const** float3_64 *unitField*)

HDINLINE float3_X picongpu::FieldBackgroundE::operator()(const DataSpace < sim
Specify your background field E(r,t) here.

Parameters

- `cellIdx`: The total cell id counted from the start at t = 0
- `currentStep`: The current time step

Public Static Attributes

constexpr bool **InfluenceParticlePusher** = false

class FieldBackgroundJ

Public Functions

PMACC_ALIGN(m_unitField, **const** float3_64)

HDINLINE **FieldBackgroundJ**(**const** float3_64 *unitField*)

HDINLINE float3_X picongpu::FieldBackgroundJ::operator()(const DataSpace < sim
Specify your background field J(r,t) here.

Parameters

- `cellIdx`: The total cell id counted from the start at t=0
- `currentStep`: The current time step

Public Static Attributes

constexpr bool **activated** = false

bremsstrahlung.param

namespace picongpu

namespace particles

namespace bremsstrahlung

namespace electron
params related to the energy loss and deflection of the incident electron

Variables

constexpr float_64 **MIN_ENERGY_MeV** = 0.5
Minimal kinetic electron energy in MeV for the lookup table.

For electrons below this value Bremsstrahlung is not taken into account.

constexpr float_64 **MAX_ENERGY_MeV** = 200.0
Maximal kinetic electron energy in MeV for the lookup table.

Electrons above this value cause a out-of-bounds access at the lookup table. Bounds checking is enabled for "CRITICAL" log level.

constexpr float_64 **MIN_THETA** = 0.01
Minimal polar deflection angle due to screening.

See Jackson 13.5 for a rule of thumb to this value.

constexpr uint32_t **NUM_SAMPLES_KAPPA** = 32
number of lookup table divisions for the kappa axis.

Kappa is the energy loss normalized to the initial kinetic energy. The axis is scaled linearly.

constexpr uint32_t **NUM_SAMPLES_EKIN** = 32
number of lookup table divisions for the initial kinetic energy axis.

The axis is scaled logarithmically.

constexpr float_64 **MIN_KAPPA** = 1.0e-10
Kappa is the energy loss normalized to the initial kinetic energy.

This minimal value is needed by the numerics to avoid a division by zero.

namespace photon
params related to the creation and the emission angle of the photon

Variables

constexpr float_64 **SOFT_PHOTONS_CUTOFF_keV** = 5000.0
Low-energy threshold in keV of the incident electron for the creation of photons.

Below this value photon emission is neglected.

constexpr uint32_t **NUM_SAMPLES_DELTA** = 256
number of lookup table divisions for the delta axis.

Delta is the angular emission probability (normalized to one) integrated from zero to theta, where theta is the angle between the photon momentum and the final electron momentum.

The axis is scaled linearly.

constexpr uint32_t **NUM_SAMPLES_GAMMA** = 64
number of lookup table divisions for the gamma axis.

Gamma is the relativistic factor of the incident electron.

The axis is scaled logarithmically.

constexpr float_64 **MAX_DELTA** = 0.95
Maximal value of delta for the lookup table.

Delta is the angular emission probability (normalized to one) integrated from zero to theta, where theta is the angle between the photon momentum and the final electron momentum.

A value close to one is reasonable. Though exactly one was actually correct, because it would map to theta = pi (maximum polar angle), the sampling then would be bad in the ultrarelativistic case. In this regime the emission primarily takes place at small thetas. So a maximum delta close to one maps to a reasonable maximum theta.

constexpr float_64 **MIN_GAMMA** = 1.0
minimal gamma for the lookup table.

constexpr float_64 **MAX_GAMMA** = 250
maximal gamma for the lookup table.

Bounds checking is enabled for “CRITICAL” log level.

constexpr float_64 **SINGLE_EMISSION_PROB_LIMIT** = 0.4
if the emission probability per timestep is higher than this value and the log level is set to “CRITICAL” a warning will be raised.

constexpr float_64 **WEIGHTING_RATIO** = 10

synchrotronPhotons.param

Defines

ENABLE_SYNCHROTRON_PHOTONS
enable synchrotron photon emission

namespace picongpu

namespace particles

namespace synchrotronPhotons

Variables

constexpr bool **enableQEDTerm** = false
enable (disable) QED (classical) photon emission spectrum

constexpr float_64 **SYNC_FUNCS_CUTOFF** = 5.0
Above this value (to the power of three, see comments on mapping) the synchrotron functions are nearly zero.

constexpr float_64 **SYNC_FUNCS_BESSEL_INTEGRAL_STEPWIDTH** = 1.0e-3
stepwidth for the numerical integration of the bessel function for the first synchrotron function

constexpr uint32_t **SYNC_FUNCS_NUM_SAMPLES** = 8192
Number of sampling points of the lookup table.

constexpr float_64 **SOFT_PHOTONS_CUTOFF_RATIO** = 1.0
Photons of oscillation periods greater than a timestep are not created since the grid already accounts for them.

This cutoff ratio is defined as: photon-oscillation-period / timestep

constexpr float_64 **SINGLE_EMISSION_PROB_LIMIT** = 0.4
if the emission probability per timestep is higher than this value and the log level is set to "CRITICAL" a warning will be raised.

ionizer.param

This file contains the proton and neutron numbers of commonly used elements of the periodic table.

The elements here should have a matching list of ionization energies in Furthermore there are parameters for specific ionization models to be found here. That includes lists of screened nuclear charges as seen by bound electrons for the aforementioned elements as well as fitting parameters of the Thomas-Fermi ionization model.

See ionizationEnergies.param. Moreover this file contains a description of how to configure an ionization model for a species.

namespace picongpu

namespace ionization
Ionization Model Configuration.

- None : no particle is ionized
- BSI : simple barrier suppression ionization
- BSIEffectiveZ : BSI taking electron shielding into account via an effective atomic number Z_eff
- ADKLinPol : Ammosov-Delone-Krainov tunneling ionization (H-like) -> linearly polarized lasers

- ADKCircPol : Ammosov-Delone-Krainov tunneling ionization (H-like) -> circularly polarized lasers
- Keldysh : Keldysh ionization model
- ThomasFermi : statistical impact ionization based on Thomas-Fermi atomic model Attention: requires 2 *FieldTmp* slots Research and development:

  See memory.param
- BSIStarkShifted : BSI for hydrogen-like atoms and ions considering the Stark upshift of ionization potentials

Usage: Add flags to the list of particle flags that has the following structure

```
   ionizers< MakeSeq_t< particles::ionization::IonizationModel<␣
↪Species2BCreated > > >,
   atomicNumbers< ionization::atomicNumbers::Element_t >,
   effectiveNuclearCharge< ionization::effectiveNuclearCharge::Element_t >
↪,
   ionizationEnergies< ionization::energies::AU::Element_t >
```

namespace atomicNumbers
Specify (chemical) element

Proton and neutron numbers define the chemical element that the ion species is based on. This value can be non-integer for physical models taking charge shielding effects into account. It is wrapped into a struct because of C++ restricting floats from being template arguments.

See http://en.wikipedia.org/wiki/Effective_nuclear_charge

Do not forget to set the correct mass and charge via `massRatio<>` and `chargeRatio<>`!

struct Aluminium_t
Al-27 ~100% NA.

Public Static Attributes

constexpr float_X **numberOfProtons** = 13.0

constexpr float_X **numberOfNeutrons** = 14.0

struct Carbon_t
C-12 98.9% NA.

Public Static Attributes

constexpr float_X **numberOfProtons** = 6.0

constexpr float_X **numberOfNeutrons** = 6.0

struct Copper_t
Cu-63 69.15% NA.

Public Static Attributes

constexpr float_X **numberOfProtons** = 29.0

constexpr float_X **numberOfNeutrons** = 34.0

struct Deuterium_t
H-2 0.02% NA.

Public Static Attributes

constexpr float_X **numberOfProtons** = 1.0

constexpr float_X **numberOfNeutrons** = 1.0

struct Gold_t
Au-197 ~100% NA.

Public Static Attributes

constexpr float_X **numberOfProtons** = 79.0

constexpr float_X **numberOfNeutrons** = 118.0

struct Helium_t
He-4 ~100% NA.

Public Static Attributes

constexpr float_X **numberOfProtons** = 2.0

constexpr float_X **numberOfNeutrons** = 2.0

struct Hydrogen_t
H-1 99.98% NA.

Public Static Attributes

constexpr float_X **numberOfProtons** = 1.0

constexpr float_X **numberOfNeutrons** = 0.0

struct Nitrogen_t
N-14 99.6% NA.

Public Static Attributes

constexpr float_X **numberOfProtons** = 7.0

constexpr float_X **numberOfNeutrons** = 7.0

struct Oxygen_t
O-16 99.76% NA.

Public Static Attributes

constexpr float_X **numberOfProtons** = 8.0

constexpr float_X **numberOfNeutrons** = 8.0

struct Silicon_t
Si-28 ~92.23% NA.

Public Static Attributes

constexpr float_X **numberOfProtons** = 14.0

constexpr float_X **numberOfNeutrons** = 14.0

namespace effectiveNuclearCharge

Effective Nuclear Charge.

Due to the shielding effect of inner electron shells in an atom / ion which makes the core charge seem smaller to valence electrons new, effective, atomic core charge numbers can be defined to make the crude barrier suppression ionization (BSI) model less inaccurate.

References: Clementi, E.; Raimondi, D. L. (1963) "Atomic Screening Constants from SCF Functions" J. Chem. Phys. 38 (11): 2686–2689. doi:10.1063/1.1733573 Clementi, E.; Raimondi, D. L.; Reinhardt, W. P. (1967) "Atomic Screening Constants from SCF Functions. II. Atoms with 37 to 86 Electrons" Journal of Chemical Physics. 47: 1300–1307. doi:10.1063/1.1712084

See https://en.wikipedia.org/wiki/Effective_nuclear_charge or refer directly to the calculations by Slater or Clementi and Raimondi

IMPORTANT NOTE: You have to insert the values in REVERSE order since the lowest shell corresponds to the last ionization process!

Functions

picongpu::ionization::effectiveNuclearCharge::PMACC_CONST_VECTOR(float_X, 1,

picongpu::ionization::effectiveNuclearCharge::PMACC_CONST_VECTOR(float_X, 1,

picongpu::ionization::effectiveNuclearCharge::PMACC_CONST_VECTOR(float_X, 2,

picongpu::ionization::effectiveNuclearCharge::PMACC_CONST_VECTOR(float_X, 6,

picongpu::ionization::effectiveNuclearCharge::PMACC_CONST_VECTOR(float_X, 7,

picongpu::ionization::effectiveNuclearCharge::PMACC_CONST_VECTOR(float_X, 8,

picongpu::ionization::effectiveNuclearCharge::PMACC_CONST_VECTOR(float_X, 13

picongpu::ionization::effectiveNuclearCharge::PMACC_CONST_VECTOR(float_X, 14

picongpu::ionization::effectiveNuclearCharge::PMACC_CONST_VECTOR(float_X, 29

picongpu::ionization::effectiveNuclearCharge::PMACC_CONST_VECTOR(float_X, 79

namespace particles

namespace ionization

namespace thomasFermi

Variables

constexpr float_X **TFAlpha** = 14.3139

Fitting parameters to average ionization degree Z* = 4/3*pi*R_0^3 * n(R_0) as an extension towards arbitrary atoms and temperatures.

See table IV of http://www.sciencedirect.com/science/article/pii/S0065219908601451 doi:10.1016/S0065-2199(08)60145-1

constexpr float_X **TFBeta** = 0.6624

constexpr float_X **TFA1** = 3.323e-3

constexpr float_X **TFA2** = 9.718e-1

constexpr float_X **TFA3** = 9.26148e-5

constexpr float_X **TFA4** = 3.10165

constexpr float_X **TFB0** = -1.7630

constexpr float_X **TFB1** = 1.43175

constexpr float_X **TFB2** = 0.31546

constexpr float_X **TFC1** = -0.366667

constexpr float_X **TFC2** = 0.983333

constexpr float_X **CUTOFF_MAX_ENERGY_KEV** = 50.0
cutoff energy for electron "temperature" calculation

In laser produced plasmas we can have different, well-separable groups of electrons. For the Thomas-Fermi ionization model we only want the thermalized "bulk" electrons. Including the high-energy "prompt" electrons is physically questionable since they do not have a large cross section for collisional ionization.

unit: keV

constexpr float_X **CUTOFF_MAX_ENERGY** = *CUTOFF_MAX_ENERGY_KEV * UNITCONV_keV_to_J*
cutoff energy for electron "temperature" calculation in SI units

constexpr float_X **CUTOFF_LOW_DENSITY** = 1.7422e27
lower ion density cutoff

The Thomas-Fermi model yields unphysical artifacts for low ion densities. Low ion densities imply lower collision frequency and thus less collisional ionization. The Thomas-Fermi model yields an increasing charge state for decreasing densities and electron temperatures of 10eV and above. This cutoff will be used to set the lower application threshold for charge state calculation.

unit: 1 / m^3
Note This cutoff value should be set in accordance to FLYCHK calculations, for instance! It is not a universal value and requires some preliminary approximations!
example: 1.7422e27 as a hydrogen ion number density equal to the corresponding critical electron number density for an 800nm laser

The choice of the default is motivated by by the following: In laser-driven plasmas all dynamics in density regions below the critical electron density will be laser-dominated. Once ions of that density are ionized once the laser will not penetrate fully anymore and the as electrons are heated the dynamics will be collision-dominated.

constexpr float_X **CUTOFF_LOW_TEMPERATURE_EV** = 1.0
lower electron temperature cutoff

The Thomas-Fermi model predicts initial ionization for many materials of solid density even when the electron temperature is 0.

ionizationEnergies.param

This file contains the ionization energies of commonly used elements of the periodic table.

Each atomic species in PIConGPU can represent exactly one element. The ionization energies of that element are stored in a vector which contains the *name* and *proton number* as well as a list of *energy values*. The number of ionization levels must be equal to the proton number of the element.

namespace picongpu

namespace ionization

Ionization Model Configuration.

- None : no particle is ionized
- BSI : simple barrier suppression ionization
- BSIEffectiveZ : BSI taking electron shielding into account via an effective atomic number Z_eff
- ADKLinPol : Ammosov-Delone-Krainov tunneling ionization (H-like) -> linearly polarized lasers
- ADKCircPol : Ammosov-Delone-Krainov tunneling ionization (H-like) -> circularly polarized lasers
- Keldysh : Keldysh ionization model
- ThomasFermi : statistical impact ionization based on Thomas-Fermi atomic model Attention: requires 2 *FieldTmp* slots Research and development:

  See memory.param
- BSIStarkShifted : BSI for hydrogen-like atoms and ions considering the Stark upshift of ionization potentials

Usage: Add flags to the list of particle flags that has the following structure

```
  ionizers< MakeSeq_t< particles::ionization::IonizationModel<␣
↪Species2BCreated > > >,
  atomicNumbers< ionization::atomicNumbers::Element_t >,
  effectiveNuclearCharge< ionization::effectiveNuclearCharge::Element_t >
↪,
  ionizationEnergies< ionization::energies::AU::Element_t >
```

namespace energies

Ionization potentials.

Please follow these rules for defining ionization energies of atomic species, unless your chosen ionization model requires a different unit system than `AU::`

- input of values in either atomic units or converting eV or Joule to them -> use either UNITCONV_eV_to_AU or SI::ATOMIC_UNIT_ENERGY for that purpose
- use `float_X` as the preferred data type

example: ionization energy for ground state hydrogen: 13.6 eV 1 Joule = 1 kg * m^2 / s^2 1 eV = 1.602e-19 J

1 AU (energy) = 27.2 eV = 1 Hartree = 4.36e-18 J = 2 Rydberg = 2 x Hydrogen ground state binding energy

Atomic units are useful for ionization models because they simplify the formulae greatly and provide intuitively understandable relations to a well-known system, i.e. the Hydrogen atom.

for PMACC_CONST_VECTOR usage, Reference: Kramida, A., Ralchenko, Yu., Reader, J., and NIST ASD Team (2014) NIST Atomic Spectra Database (ver. 5.2), [Online] Available: http://physics.nist.gov/asd [2017, February 8] National Institute of Standards and Technology, Gaithersburg, MD

See include/pmacc/math/ConstVector.hpp for finding ionization energies, http://physics.nist.gov/PhysRefData/ASD/ionEnergy.html

namespace AU

Functions

picongpu::ionization::energies::AU::PMACC_CONST_VECTOR(float_X, 1, Hydrog

picongpu::ionization::energies::AU::PMACC_CONST_VECTOR(float_X, 1, Deuter

picongpu::ionization::energies::AU::PMACC_CONST_VECTOR(float_X, 2, Heliu

picongpu::ionization::energies::AU::PMACC_CONST_VECTOR(float_X, 6, Carbo

picongpu::ionization::energies::AU::PMACC_CONST_VECTOR(float_X, 7, Nitrog

picongpu::ionization::energies::AU::PMACC_CONST_VECTOR(float_X, 8, Oxyge

picongpu::ionization::energies::AU::PMACC_CONST_VECTOR(float_X, 13, Alumi

picongpu::ionization::energies::AU::PMACC_CONST_VECTOR(float_X, 14, Silic

picongpu::ionization::energies::AU::PMACC_CONST_VECTOR(float_X, 29, Coppe

picongpu::ionization::energies::AU::PMACC_CONST_VECTOR(float_X, 79, Gold,

flylite.param

This is the configuration file for the atomic particle population kinetics model FLYlite.

Its main purpose is non-LTE collisional-radiative modeling for transient plasmas at high densities and/or interaction with (X-Ray) photon fields.

In simpler words, one can also use this module to simulate collisional ionization processes without the assumption of a local thermal equilibrium (LTE), contrary to popular collisional ionization models such as the Thomas-Fermi ionization model.

This file configures the number of modeled populations for ions, spatial and spectral binning of non-LTE density and energy histograms.

namespace picongpu

namespace flylite

Typedefs

using Superconfig = types::Superconfig<float_64, *populations*>

using spatialAverageBox = *SuperCellSize*
you better not change this line, the wooooorld depends on it!

no seriously, per-supercell is the quickest way to average particle quantities such as density, energy histogram, etc. and I won't implement another size until needed

Variables

constexpr uint8_t **populations** = 3u
number of populations (numpop)

this number defines how many configurations make up a superconfiguration

range: [0, 255]

constexpr uint8_t **ionizationStates** = 29u
ionization states of the atom (iz)

range: [0, 255]

constexpr uint16_t **energies** = 512u
number of energy bins

energy steps used for local energy histograms

Note : no overflow- or underflow-bins are used, particles with energies outside the range (see below) are ignored

constexpr float_X **electronMinEnergy** = 0.0
energy range for electron and photon histograms

electron and photon histograms f(e) f(ph) are currently calculated in a linearly binned histogram while particles with energies outside the ranges below are ignored

unit: eV

constexpr float_X **electronMaxEnergy** = 100.e3

constexpr float_X **photonMinEnergy** = 0.0

constexpr float_X **photonMaxEnergy** = 100.e3

collision.param

namespace picongpu

namespace particles

namespace collision

Typedefs

using CollisionPipeline = bmpl::vector<>
CollisionPipeline defines in which order species interact with each other.

the functors are called in order (from first to last functor)

namespace precision

Typedefs

using float_COLL = float_64

More information on collision.param

Plugins

fileOutput.param

namespace picongpu

Typedefs

using ChargeDensity_Seq = deriveField::CreateEligible_t<*VectorAllSpecies*, deriveField::derivedAttributes::ChargeD
FieldTmp output (calculated at runtime) ********************************.

Those operations derive scalar field quantities from particle species at runtime. Each value is mapped per cell. Some operations are identical up to a constant, so avoid writing those twice to save storage.

you can choose any of these particle to grid projections:

- Density: particle position + shape on the grid
- BoundElectronDensity: density of bound electrons note: only makes sense for partially ionized ions
- ChargeDensity: density * charge note: for species that do not change their charge state, this is the same as the density times a constant for the charge
- Energy: sum of kinetic particle energy per cell with respect to shape
- EnergyDensity: average kinetic particle energy per cell times the particle density note: this is the same as the sum of kinetic particle energy divided by a constant for the cell volume
- MomentumComponent: ratio between a selected momentum component and the absolute momentum with respect to shape
- LarmorPower: radiated Larmor power (species must contain the attribute `momentumPrev1`)

for debugging:

- MidCurrentDensityComponent: density * charge * velocity_component
- Counter: counts point like particles per cell
- MacroCounter: counts point like macro particles per cell

Filtering: You can create derived fields from filtered particles. Only particles passing the filter will contribute to the field quantity. For that you need to define your filters in `particleFilters.param` and pass a filter as the 3rd (optional) template argument in `CreateEligible_t`.

Example: This will create charge density field for all species that are eligible for the this attribute and the chosen filter.

```
using ChargeDensity_Seq
= deriveField::CreateEligible_t< VectorAllSpecies,
deriveField::derivedAttributes::ChargeDensity, filter::FilterOfYourChoice>
↪;
```

using EnergyDensity_Seq = deriveField::CreateEligible_t<*VectorAllSpecies*, deriveField::derivedAttributes::EnergyI

using MomentumComponent_Seq = deriveField::CreateEligible_t<*VectorAllSpecies*, deriveField::derivedAttributes::M

using FieldTmpSolvers = MakeSeq_t<*ChargeDensity_Seq*, *EnergyDensity_Seq*, *MomentumComponent_Seq*>
FieldTmpSolvers groups all solvers that create data for *FieldTmp* ******.

FieldTmpSolvers is used in

See *FieldTmp* to calculate the exchange size

using NativeFileOutputFields = MakeSeq_t<*FieldE*, *FieldB*>
FileOutputFields: Groups all Fields that shall be dumped.

Possible native fields: *FieldE*, *FieldB*, *FieldJ*

using FileOutputFields = MakeSeq_t<*NativeFileOutputFields*, *FieldTmpSolvers*>

using FileOutputParticles = *VectorAllSpecies*
FileOutputParticles: Groups all Species that shall be dumped **********.

hint: to disable particle output set to using FileOutputParticles = MakeSeq_t< >;

isaac.param

Definition which native fields and density fields of (filtered) particles will be visualizable with ISAAC.

ISAAC is an in-situ visualization library with which the PIC simulation can be observed while it is running avoiding the time consuming writing and reading of simulation data for the classical post processing of data.

ISAAC can directly visualize natives fields like the E or B field, but density fields of particles need to be calculated from PIConGPU on the fly which slightly increases the runtime and the memory consumption. Every particle density field will reduce the amount of memory left for PIConGPUs particles and fields.

To get best performance, ISAAC defines an exponential amount of different visualization kernels for every combination of (at runtime) activated fields. So furthermore a lot of fields will increase the compilation time.

namespace picongpu

namespace isaacP

Typedefs

using Particle_Seq = *VectorAllSpecies*
Intermediate list of native particle species of PIConGPU which shall be visualized.

using Native_Seq = MakeSeq_t<*FieldE*, *FieldB*, *FieldJ*>
Intermediate list of native fields of PIConGPU which shall be visualized.

using Density_Seq = deriveField::CreateEligible_t<*Particle_Seq*, deriveField::derivedAttributes::Density>
Intermediate list of particle species, from which density fields shall be created at runtime to visualize them.

You can create such densities from filtered particles by passing a particle filter as the third template argument (`filter::All` by default). Don't forget to add your filtered densities to the `Fields_Seq` below.

```
using Density_Seq_Filtered = deriveField::CreateEligible_t<Particle_
↪Seq,
    deriveField::derivedAttributes::Density, filter::All>;
```

using Fields_Seq = MakeSeq_t<*Native_Seq*, *Density_Seq*>
Compile time sequence of all fields which shall be visualized.

Basically joining Native_Seq and Density_Seq.

using VectorFields_Seq = *Native_Seq*
Compile time sequence of all fields which shall be visualized.

Basically joining Native_Seq and Density_Seq.

particleCalorimeter.param

namespace picongpu

namespace particleCalorimeter

Functions

HDINLINE float2_X picongpu::particleCalorimeter::mapYawPitchToNormedRange(const
Map yaw and pitch into [0,1] respectively.

These ranges correspond to the normalized histogram range of the calorimeter (0: first bin, 1: last bin). Out-of-range values are mapped to the first or the last bin.

Useful for fine tuning the spatial calorimeter resolution.

Return Two values within [-1,1]

Parameters

- `yaw`: -maxYaw. . . maxYaw
- `pitch`: -maxPitch. . . maxPitch
- `maxYaw`: maximum value of angle yaw
- `maxPitch`: maximum value of angle pitch

particleMerger.param

namespace picongpu

namespace plugins

namespace particleMerging

Variables

constexpr size_t **MAX_VORONOI_CELLS** = 128
maximum number of active Voronoi cells per supercell.

If the number of active Voronoi cells reaches this limit merging events are dropped.

radiation.param

Definition of frequency space, number of observers, filters, form factors and window functions of the radiation plugin.

All values set here determine what the radiation plugin will compute. The observation direction is defined in a seperate file `radiationObserver.param`. On the comand line the plugin still needs to be called for each species the radiation should be computed for.

Defines

PIC_VERBOSE_RADIATION
radiation verbose level: 0=nothing, 1=physics, 2=simulation_state, 4=memory, 8=critical

namespace picongpu

namespace plugins

namespace radiation

Typedefs

using RadiationParticleFilter = *picongpu*::*particles*::*manipulators*::generic::*Free*<*GammaFilterFu*
filter to (de)select particles for the radiation calculation

to activate the filter:
- goto file `speciesDefinition.param`
- add the attribute `radiationMask` to the particle species

struct GammaFilterFunctor
select particles for radiation example of a filter for the relativistic Lorentz factor gamma

Public Functions

template<typename T_Particle>HDINLINE void picongpu::plugins::radiation::

Public Static Attributes

constexpr float_X **radiationGamma** = 5.0
Gamma value above which the radiation is calculated.

namespace frequencies_from_list

Variables

constexpr const char ***listLocation** = "/path/to/frequency_list"
path to text file with frequencies

constexpr unsigned int **N_omega** = 2048
number of frequency values to compute if frequencies are given in a file [unitless]

namespace linear_frequencies

Variables

constexpr unsigned int **N_omega** = 2048
number of frequency values to compute in the linear frequency [unitless]

namespace SI

Variables

constexpr float_64 **omega_min** = 0.0
mimimum frequency of the linear frequency scale in units of [1/s]

constexpr float_64 **omega_max** = 1.06e16
maximum frequency of the linear frequency scale in units of [1/s]

namespace log_frequencies

Variables

constexpr unsigned int **N_omega** = 2048
number of frequency values to compute in the logarithmic frequency [unitless]

namespace SI

Variables

constexpr float_64 **omega_min** = 1.0e14
mimimum frequency of the logarithmic frequency scale in units of [1/s]

constexpr float_64 **omega_max** = 1.0e17
maximum frequency of the logarithmic frequency scale in units of [1/s]

namespace parameters

Variables

constexpr unsigned int **N_observer** = 256
number of observation directions

namespace radFormFactor_CIC_3D
correct treatment of coherent and incoherent radiation from macro particles

Choose different form factors in order to consider different particle shapes for radiation
- radFormFactor_CIC_3D ... CIC charge distribution
- radFormFactor_TSC_3D ... TSC charge distribution
- radFormFactor_PCS_3D ... PCS charge distribution
- radFormFactor_CIC_1Dy ... only CIC charge distribution in y
- radFormFactor_Gauss_spherical ... symmetric Gauss charge distribution
- radFormFactor_Gauss_cell ... Gauss charge distribution according to cell size
- radFormFactor_incoherent ... only incoherent radiation
- radFormFactor_coherent ... only coherent radiation

namespace radiationNyquist
selected mode of frequency scaling:

options:
- linear_frequencies
- log_frequencies
- frequencies_from_list

Variables

constexpr float_32 **NyquistFactor** = 0.5
Nyquist factor: fraction of the local Nyquist frequency above which the spectra is set to zero should be in (0, 1).

namespace radWindowFunctionTriangle
add a window function weighting to the radiation in order to avoid ringing effects from sharpe boundaries default: no window function via `radWindowFunctionNone`

Choose different window function in order to get better ringing reduction radWindowFunctionTriangle radWindowFunctionHamming radWindowFunctionTriplett radWindowFunctionGauss radWindowFunctionNone

radiationObserver.param

This file defines a function describing the observation directions.

It takes an integer index from [0, picongpu::parameters::N_observer) and maps it to a 3D unit vector in R^3 (norm=1) space that describes the observation direction in the PIConGPU cartesian coordinate system.

namespace picongpu

namespace plugins

namespace radiation

namespace radiation_observer

Functions

HDINLINE vector_64 picongpu::plugins::radiation::radiation_observer::obse

Compute observation angles.

This function is used in the Radiation plug-in kernel to compute the observation directions given as a unit vector pointing towards a 'virtual' detector

This default setup is an example of a 2D detector array. It computes observation directions for 2D virtual detector field with its center pointing toward the +y direction (for theta=0, phi=0) with observation angles ranging from theta = [angle_theta_start : angle_theta_end] phi = [angle_phi_start : angle_phi_end] Every observation_id_extern index moves the phi angle from its start value toward its end value until the observation_id_extern reaches N_split. After that the theta angle moves further from its start value towards its end value while phi is reset to its start value.

The unit vector pointing towards the observing virtual detector can be described using theta and phi by: x_value = sin(theta) * cos(phi) y_value = cos(theta) z_value = sin(theta) * sin(phi) These are the standard spherical coordinates.

The example setup describes an detector array of 16x16 detectors ranging from -pi/8= -22.5 degrees to +pi/8= +22.5 degrees for both angles with the center pointing toward the y-axis (laser propagation direction).

Return unit vector pointing in observation direction type: vector_64

Parameters

- `observation_id_extern`: int index that identifies each block on the GPU to compute the observation direction

png.param

Defines

EM_FIELD_SCALE_CHANNEL1

EM_FIELD_SCALE_CHANNEL2

EM_FIELD_SCALE_CHANNEL3

namespace picongpu

Variables

constexpr float_64 **scale_image** = 1.0

constexpr bool **scale_to_cellsize** = true

constexpr bool **white_box_per_GPU** = false

namespace visPreview

Functions

DINLINE float_X picongpu::visPreview::preChannel1(const float3_X & field_B, c

DINLINE float_X picongpu::visPreview::preChannel2(const float3_X & field_B, c

DINLINE float_X picongpu::visPreview::preChannel3(const float3_X & field_B, c

Variables

```
constexpr float_X picongpu::visPreview::preParticleDens_opacity = 0.25_X
constexpr float_X picongpu::visPreview::preChannel1_opacity = 1.0_X
constexpr float_X picongpu::visPreview::preChannel2_opacity = 1.0_X
constexpr float_X picongpu::visPreview::preChannel3_opacity = 1.0_X
```

pngColorScales.param

```
namespace picongpu

    namespace colorScales

        namespace blue
```

Functions

```
HDINLINE void picongpu::colorScales::blue::addRGB(float3_X  & img, const flo
```

```
        namespace gray
```

Functions

```
HDINLINE void picongpu::colorScales::gray::addRGB(float3_X  & img, const flo
```

```
        namespace grayInv
```

Functions

```
HDINLINE void picongpu::colorScales::grayInv::addRGB(float3_X  & img, const
```

```
        namespace green
```

Functions

```
HDINLINE void picongpu::colorScales::green::addRGB(float3_X  & img, const fl
```

```
        namespace none
```

Functions

```
HDINLINE void picongpu::colorScales::none::addRGB(const  float3_X  &, const
```

```
        namespace red
```

Functions

```
HDINLINE void picongpu::colorScales::red::addRGB(float3_X  & img, const floa
```

transitionRadiation.param

Definition of frequency space, number of observers, filters and form factors of the transition radiation plugin.

All values set here determine what the radiation plugin will compute. On the comand line the plugin still needs to be called for each species the transition radiation should be computed for.

Defines

PIC_VERBOSE_RADIATION
Uses the same verbose level schemes as the radiation plugin.

radiation verbose level: 0=nothing, 1=physics, 2=simulation_state, 4=memory, 8=critical

namespace picongpu

namespace plugins

namespace radiation

namespace radFormFactor_CIC_3D
correct treatment of coherent and incoherent radiation from macro particles

Choose different form factors in order to consider different particle shapes for radiation
- radFormFactor_CIC_3D ... CIC charge distribution
- radFormFactor_TSC_3D ... TSC charge distribution
- radFormFactor_PCS_3D ... PCS charge distribution
- radFormFactor_CIC_1Dy ... only CIC charge distribution in y
- radFormFactor_Gauss_spherical ... symmetric Gauss charge distribution
- radFormFactor_Gauss_cell ... Gauss charge distribution according to cell size
- radFormFactor_incoherent ... only incoherent radiation
- radFormFactor_coherent ... only coherent radiation

namespace transitionRadiation

Typedefs

using GammaFilter = *picongpu*::*particles*::*manipulators*::generic::*Free*<*GammaFilterFunctor*>
filter to (de)select particles for the radiation calculation

to activate the filter:
- goto file `speciesDefinition.param`
- add the attribute `transitionRadiationMask` to the particle species

Warning Do not remove this filter. Otherwise still standing electrons would generate NaNs in the output of the plugin and transition radiation is scaling proportionally to gamma^2.

Functions

HDINLINE float3_X picongpu::plugins::transitionRadiation::observationDirecti
Compute observation angles.

This function is used in the transition radiation plugin kernel to compute the observation directions given as a unit vector pointing towards a 'virtual' detector

This default setup is an example of a 2D detector array. It computes observation directions for 2D virtual detector field with its center pointing toward the +y direction (for theta=0, phi=0) with observation angles ranging from theta = [angle_theta_start : angle_theta_end]

phi = [angle_phi_start : angle_phi_end] Every observation_id_extern index moves the phi angle from its start value toward its end value until the observation_id_extern reaches N_split. After that the theta angle moves further from its start value towards its end value while phi is reset to its start value.

The unit vector pointing towards the observing virtual detector can be described using theta and phi by: x_value = sin(theta) * cos(phi) y_value = cos(theta) z_value = sin(theta) * sin(phi) These are the standard spherical coordinates.

The example setup describes an detector array of 128X128 detectors ranging from 0 to pi for the azimuth angle theta and from 0 to 2 pi for the polar angle phi.

If the calculation is only supposed to be done for a single azimuth or polar angle, it will use the respective minimal angle.

Return unit vector pointing in observation direction type: float3_X
Parameters

- `observation_id_extern`: int index that identifies each block on the GPU to compute the observation direction

struct GammaFilterFunctor
example of a filter for the relativistic Lorentz factor gamma

Public Functions

template<typename T_Particle>HDINLINE void picongpu::plugins::transitionR

Public Static Attributes

constexpr float_X **filterGamma** = 5.0
Gamma value above which the radiation is calculated, must be positive.

namespace linearFrequencies
units for linear frequencies distribution for transition radiation plugin

Variables

constexpr unsigned int **nOmega** = 512
number of frequency values to compute in the linear frequency [unitless]

namespace SI

Variables

constexpr float_64 **omegaMin** = 0.0
mimimum frequency of the linear frequency scale in units of [1/s]

constexpr float_64 **omegaMax** = 1.06e16
maximum frequency of the linear frequency scale in units of [1/s]

namespace listFrequencies
units for frequencies from list for transition radiation calculation

Variables

constexpr char **listLocation**[] = "/path/to/frequency_list"
path to text file with frequencies

constexpr unsigned int **nOmega** = 512
number of frequency values to compute if frequencies are given in a file [unitless]

namespace logFrequencies
units for logarithmic frequencies distribution for transition radiation plugin

Variables

constexpr unsigned int **nOmega** = 256
number of frequency values to compute in the logarithmic frequency [unitless]

namespace SI

Variables

constexpr float_64 **omegaMin** = 1.0e13
mimimum frequency of the logarithmic frequency scale in units of [1/s]

constexpr float_64 **omegaMax** = 1.0e17
maximum frequency of the logarithmic frequency scale in units of [1/s]

namespace parameters
selected mode of frequency scaling:

unit for foil position

options:
- linearFrequencies
- logFrequencies
- listFrequencies correct treatment of coherent radiation from macro particles

These formfactors are the same as in the radiation plugin! Choose different form factors in order to consider different particle shapes for radiation
- picongpu::plugins::radiation::radFormFactor_CIC_3D ... CIC charge distribution
- ::picongpu::plugins::radiation::radFormFactor_TSC_3D ... TSC charge distribution
- ::picongpu::plugins::radiation::radFormFactor_PCS_3D ... PCS charge distribution
- ::picongpu::plugins::radiation::radFormFactor_CIC_1Dy ... only CIC charge distribution in y
- ::picongpu::plugins::radiation::radFormFactor_Gauss_spherical ... symmetric Gauss charge distribution
- ::picongpu::plugins::radiation::radFormFactor_Gauss_cell ... Gauss charge distribution according to cell size
- ::picongpu::plugins::radiation::radFormFactor_incoherent ... only incoherent radiation
- ::picongpu::plugins::radiation::radFormFactor_coherent ... only coherent radiation

Variables

constexpr unsigned int **nPhi** = 128
Number of observation directions.

If nPhi or nTheta is equal to 1, the transition radiation will be calculated for phiMin or thetaMin respectively.

constexpr unsigned int **nTheta** = 128

constexpr unsigned int **nObserver** = *nPhi * nTheta*

constexpr float_64 **thetaMin** = 0.0

constexpr float_64 **thetaMax** = *picongpu*::*PI*

constexpr float_64 **phiMin** = 0.0

constexpr float_64 **phiMax** = 2 * *picongpu*::*PI*

namespace SI

Variables

constexpr float_64 **foilPosition** = 0.0

Misc

starter.param

random.param

Configure the pseudorandom number generator (PRNG).

Allows to select method and global seeds in order to vary the initial state of the parallel PRNG.

namespace picongpu

namespace random

Typedefs

using Generator = *pmacc*::random::methods::XorMin<>
Random number generation methods.

It is not allowed to change the method and restart an already existing checkpoint.

- pmacc::random::methods::XorMin
- pmacc::random::methods::MRG32k3aMin
- pmacc::random::methods::AlpakaRand

using SeedGenerator = seed::Value<42>
random number start seed

Generator to create a seed for the random number generator. Depending of the generator the seed is reproducible or or changed with each program execution.

- seed::Value< 42 >
- seed::FromTime
- seed::FromEnvironment

physicalConstants.param

namespace picongpu

Variables

constexpr float_64 **PI** = 3.14159265358979323846264338327950288419716939937

constexpr float_64 **UNIT_SPEED** = *SI*::*SPEED_OF_LIGHT_SI*
Unit of speed.

constexpr float_X **SPEED_OF_LIGHT** = float_X(*SI*::*SPEED_OF_LIGHT_SI* / *UNIT_SPEED*)

constexpr float_64 **UNITCONV_keV_to_Joule** = 1.60217646e-16

constexpr float_64 **UNITCONV_Joule_to_keV** = (1.0 / *UNITCONV_keV_to_Joule*)

constexpr float_64 **UNITCONV_AU_to_eV** = 27.21139

constexpr float_64 **UNITCONV_eV_to_AU** = (1.0 / *UNITCONV_AU_to_eV*)

namespace SI

Variables

constexpr float_64 **SPEED_OF_LIGHT_SI** = 2.99792458e8
unit: m / s

constexpr float_64 **MUE0_SI** = *PI* * 4.e-7
unit: N / A^2

constexpr float_64 **EPS0_SI** = 1.0 / *MUE0_SI* / *SPEED_OF_LIGHT_SI* / *SPEED_OF_LIGHT_SI*
unit: C / (V m)

constexpr float_64 **Z0_SI** = *MUE0_SI* * *SPEED_OF_LIGHT_SI*
impedance of free space unit: ohm

constexpr float_64 **HBAR_SI** = 1.054571800e-34
reduced Planck constant unit: J * s

constexpr float_64 **ELECTRON_MASS_SI** = 9.109382e-31
unit: kg

constexpr float_64 **ELECTRON_CHARGE_SI** = -1.602176e-19
unit: C

constexpr float_64 **ATOMIC_UNIT_ENERGY** = 4.36e-18

constexpr float_64 **ATOMIC_UNIT_EFIELD** = 5.14e11

constexpr float_64 **ATOMIC_UNIT_TIME** = 2.4189e-17

constexpr float_64 **N_AVOGADRO** = 6.02214076e23
Avogadro number unit: mol^-1.

Y. Azuma et al. Improved measurement results for the Avogadro constant using a 28-Si-enriched crystal, Metrologie 52, 2015, 360-375 doi:10.1088/0026-1394/52/2/360

constexpr float_64 **ELECTRON_RADIUS_SI** = *ELECTRON_CHARGE_SI* * *ELECTRON_CHARGE_SI* / (4.0 * *P*
Classical electron radius in SI units.

2.3.5 Python Generator (Third party)

PoGit is a utility to generate a set of `.param files` and a `.cfg` file using a Pythonic API. PoGit is a third-party development and supports only a subset of PIConGPU compile- and run-time settings. However, the resulting output can serve as a basis to be edited as normal `.param files`.

2.4 Plugins

Plugin name	short description
openPMD[26]	outputs simulation data via the openPMD API
energy histogram[6]	energy histograms for electrons and ions
charge conservation[5]	maximum difference between electron charge density and div E
checkpoint[2]	stores the primary data of the simulation for restarts.
count particles[5]	count total number of macro particles
count per supercell[2]	count macro particles *per supercell*
energy fields	electromagnetic field energy per time step
energy particles[6]	kinetic and total energies summed over all electrons and/or ions
ISAAC	interactive 3D live visualization [Matthes2016]
intensity[145]	maximum and integrated electric field along the y-direction
particle calorimeter[236]	spatially resolved, particle energy detector in infinite distance
particle merger[5]	macro particle merging
phase space[256]	calculate 2D phase space [Huebl2014]
PNG[6]	pictures of 2D slices
positions particles[145]	save trajectory, momentum, ... of a *single* particle
radiation[2]	compute emitted electromagnetic spectra [Pausch2012] [Pausch2014] [Pausch2018]
resource log	monitor used hardware resources & memory
slice emittance	compute emittance and slice emittance of particles
slice field printer[45]	print out a slice of the electric and/or magnetic and/or current field
sum currents[5]	compute the total current summed over all cells
transitionRadiation	compute emitted electromagnetic spectra
xrayScattering[2]	compute SAXS scattering amplitude (based on *FieldTmp* species density)

2.4.1 Charge Conservation

First the charge density of all species with respect to their shape function is computed. Then this charge density is compared to the charge density computed from the divergence of the electric field $\nabla \vec{E}$. The maximum deviation value multiplied by the cell's volume is printed.

Attention: This plugin assumes a Yee-like divergence E stencil!

.cfg file

PIConGPU command line argument (for `.cfg` files):

```
--chargeConservation.period <periodOfSteps>
```

Memory Complexity

Accelerator

no extra allocations (needs at least one FieldTmp slot).

[2] Requires PIConGPU to be compiled with openPMD API.
[6] Multi-Plugin: Can be configured to run multiple times with varying parameters.
[5] Only runs on the *CUDA* backend (GPU).
[1] On restart, plugins with that footnote overwrite their output of previous runs. Manually *save* the created files of these plugins before restarting in the same directory.
[4] Deprecated
[3] Can remember particles that left the box at a certain time step.

Host

negligible.

Output and Analysis Tools

A new file named `chargeConservation.dat` is generated:

```
#timestep max-charge-deviation unit[As]
0 7.59718e-06 5.23234e-17
100 8.99187e-05 5.23234e-17
200 0.000113926 5.23234e-17
300 0.00014836 5.23234e-17
400 0.000154502 5.23234e-17
500 0.000164952 5.23234e-17
```

The charge is normalized to `UNIT_CHARGE` (third column) which is the typical charge of *one* macro-particle.

There is a up 5% difference to a native hdf5 post-processing based implementation of the charge conversation check due to a different order of subtraction. And the zero-th time step (only numerical differences) might differ more then 5% relative due to the close to zero result.

Known Limitations

- this plugin is only available with the CUDA backend

2.4.2 Checkpoint

Stores the primary data of the simulation for restarts. Primary data includes:

- electro-magnetic fields
- particle attributes
- state of random number generators and particle ID generator
- ...

Note: Some plugins have their own internal state. They will be notified on checkpoints to store their state themselves.

What is the format of the created files?

We write our fields and particles in an open markup called *openPMD*.

For further details, see *the openPMD API* section.

External Dependencies

The plugin is available as soon as the *openPMD API library* is compiled in.

.cfg file

You can use `--checkpoint.period` to specify the output period of the created checkpoints.

PIConGPU command line option	Description
`--checkpoint.period <N>`	Create checkpoints every N steps.
`--checkpoint.backend <IO-backend>`	IO-backend used to create the checkpoint.
`--checkpoint.directory <string>`	Directory inside `simOutput` for writing checkpoints. Default is `checkpoints`.
`--checkpoint.file <string>`	Relative or absolute fileset prefix for writing checkpoints. If relative, checkpoint files are stored under `simOutput/<checkpoint-directory>`. Default depends on the selected IO-backend.
`--checkpoint.restart`	Restart a simulation from the latest checkpoint (requires a valid checkpoint).
`--checkpoint.tryRestart`	Restart a simulation from the latest checkpoint if available else start from scratch.
`--checkpoint.restart.step <N>`	Select a specific restart checkpoint.
`--checkpoint.restart.backend <IO-backend>`	IO-backend used to load a existent checkpoint.
`--checkpoint.restart.directory <string>`	Directory inside `simOutput` containing checkpoints for a restart. Default is `checkpoints`.
`--checkpoint.restart.file <string>`	Relative or absolute fileset prefix for reading checkpoints. If relative, checkpoint files are searched under `simOutput/<checkpoint-directory>`. Default depends on the selected IO-backend‘‘.
`--checkpoint.restart.chunkSize <N>`	Number of particles processed in one kernel call during restart to prevent frame count blowup.
`--checkpoint.restart.loop <N>`	Number of times to restart the simulation after simulation has finished. This mode is intended for visualization and not all plugins support it.
`--checkpoint.<IO-backend>.*`	Additional options to control the IO-backend

Depending on the available external dependencies (see above), the options for the *<IO-backend>* are:

- *openPMD*

Interacting Manually with Checkpoint Data

Note: Interacting with the *raw data of checkpoints* for manual manipulation is considered an advanced feature for experienced users.

Contrary to regular output, checkpoints contain additional data which might be confusing on the first glance. For example, some comments might be missing, all data from our concept of slides for moving window simulations will be visible, additional data for internal states of helper classes is stored as well and index tables such as openPMD particle patches are essential for parallel restarts.

2.4.3 Count Particles

This plugin counts the total number of *macro particles associated with a species* and writes them to a file for specified time steps. It is used mainly for debugging purposes. Only in case of constant particle density, where each macro particle describes the same number of real particles (weighting), conclusions on the plasma density can be drawn.

.cfg file

The *CountParticles* plugin is always complied for all species. By specifying the periodicity of the output using the command line argument `--e_macroParticlesCount.period` (here for an electron species called `e`) with picongpu, the plugin is enabled. Setting `--e_macroParticlesCount.period 100` adds the number of all electron macro particles to the file *ElectronsCount.dat* for every 100th time step of the simulation.

Memory Complexity

Accelerator

no extra allocations.

Host

negligible.

Output

In the output file `e_macroParticlesCount.dat` there are three columns. The first is the integer number of the time step. The second is the number of macro particles as integer - useful for exact counts. And the third is the number of macro particles in scientific floating point notation - provides better human readability.

Known Issues

Currently, the file `e_macroParticlesCount.dat` is overwritten when restarting the simulation. Therefore, all previously stored counts are lost.

2.4.4 Count per Supercell

This plugin counts the total number of *macro particles of a species* for each super cell and stores the result in an hdf5 file. Only in case of constant particle weighting, where each macro particle describes the same number of real particles, conclusions on the plasma density can be drawn.

External Dependencies

The plugin is available as soon as the *openPMD API* is compiled in.

.cfg files

By specifying the periodicity of the output using the command line argument `--e_macroParticlesPerSuperCell.period` (here for an electron species `e`) with picongpu the plugin is enabled. Setting `--e_macroParticlesPerSuperCell.period 100` adds the number of all electron macro particles to the file `e_macroParticlesCount.dat` for every 100th time step of the simulation.

Accelerator

an extra permanent allocation of `size_t` for each local supercell.

Host

negligible.

Output

The output is stored as hdf5 file in a separate directory.

2.4.5 Energy Fields

This plugin computes the total energy contained in the electric and magnetic field of the entire volume simulated. The energy is computed for user specified time steps.

.cfg file

By setting the PIConGPU command line flag `--fields_energy.period` to a non-zero value the plugin computes the total field energy. The default value is `0`, meaning that the total field energy is not stored. By setting e.g. `--fields_energy.period 100` the total field energy is computed for time steps *0, 100, 200, ...*

Memory Complexity

Accelerator

negligible.

Host

negligible.

Output

The data is stored in `fields_energy.dat`. There are two columns. The first gives the time step. The second is the total field energy in **Joule**. The first row is a comment describing the columns:

```
#step total[Joule] Bx[Joule] By[Joule] Bz[Joule] Ex[Joule] Ey[Joule] Ez[Joule]
0     2.5e+18      0          0          0          2.5e+18   0          0
100   2.5e+18      2.45e-22   2.26e-08   2.24e-08   2.5e+18   2.29e-08   2.30e-08
```

Attention: The output of this plugin computes a *sum over all cells* in a very naive implementation. This can lead to significant errors due to the finite precision in floating-point numbers. Do not expect the output to be precise to more than a few percent. Do not expect the output to be deterministic due to the statistical nature of the implemented reduce operation.

Please see this issue for a longer discussion and possible future implementations.

Example Visualization

Python example snippet:

```
import numpy as np
import matplotlib.pyplot as plt


simDir = "path/to/simOutput/"

# Ekin in Joules (see EnergyParticles)
e_sum_ene = np.loadtxt(simDir + "e_energy_all.dat")[:, 0:2]
p_sum_ene = np.loadtxt(simDir + "p_energy_all.dat")[:, 0:2]
C_sum_ene = np.loadtxt(simDir + "C_energy_all.dat")[:, 0:2]
N_sum_ene = np.loadtxt(simDir + "N_energy_all.dat")[:, 0:2]
# Etotal in Joules
fields_sum_ene = np.loadtxt(simDir + "fields_energy.dat")[:, 0:2]

plt.figure()
plt.plot(e_sum_ene[:,0], e_sum_ene[:,1], label="e")
plt.plot(p_sum_ene[:,0], p_sum_ene[:,1], label="p")
plt.plot(C_sum_ene[:,0], C_sum_ene[:,1], label="C")
plt.plot(N_sum_ene[:,0], N_sum_ene[:,1], label="N")
plt.plot(fields_sum_ene[:,0], fields_sum_ene[:,1], label="fields")
plt.plot(
    e_sum_ene[:,0],
    e_sum_ene[:,1] + p_sum_ene[:,1] + C_sum_ene[:,1] + N_sum_ene[:,1] + fields_sum_
↪ene[:,1],
    label="sum"
)
plt.legend()
plt.show()
```

2.4.6 Energy Histogram

This plugin computes the energy histogram (spectrum) of a selected particle species and stores it to plain text files. The acceptance of particles for counting in the energy histogram can be adjusted, e.g. to model the limited acceptance of a realistic spectrometer.

.param file

The *particleFilters.param* file allows to define accepted particles for the energy histogram. A typical *filter* could select particles within a specified *opening angle in forward direction*.

.cfg files

There are several command line parameters that can be used to set up this plugin. Replace the prefix `e` for electrons with any other species you have defined, we keep using `e` in the examples below for simplicity. Currently, the plugin can be set *once for each species*.

PIConGPU command line option	description
`--e_energyHistogram.period`	The output periodicity of the **electron** histogram. A value of `100` would mean an output at simulation time step *0, 100, 200, ...*. If set to a non-zero value, the energy histogram of all **electrons** is computed. By default, the value is `0` and no histogram for the electrons is computed.
`--e_energy.filter`	Use filtered particles. Available filters are set up in *particleFilters.param*.
`--e_energyHistogram.binCount`	Specifies the number of bins used for the **electron** histogram. Default is `1024`.
`--e_energyHistogram.minEnergy`	Set the minimum energy for the **electron** histogram in *keV*. Default is `0`, meaning *0 keV*.
`--e_energyHistogram.maxEnergy`	Set the maximum energy for the **electron** histogram in *keV*. There is **no default value**. This has to be set by the user if `--e_energyHistogram.period 1` is set.

Note: This plugin is a multi plugin. Command line parameter can be used multiple times to create e.g. dumps with different dumping period. In the case where an optional parameter with a default value is explicitly defined the parameter will be always passed to the instance of the multi plugin where the parameter is not set. For example,

```
--e_energyHistogram.period 128 --e_energyHistogram.filter all --e_energyHistogram.
↪maxEnergy 10
--e_energyHistogram.period 100 --e_energyHistogram.filter all --e_energyHistogram.
↪maxEnergy 20 --e_energyHistogram.binCount 512
```

creates two plugins:

1. create an electron histogram **with 512 bins** each 128th time step.
2. create an electron histogram **with 1024 bins** (this is the default) each 100th time step.

Memory Complexity

Accelerator

an extra array with the number of bins.

Host

negligible.

Output

The histograms are stored in ASCII files in the `simOutput/` directory.

The file for the electron histogram is named `e_energyHistogram.dat` and for all other species `<species>_energyHistogram.dat` likewise. The first line of these files does not contain histogram data and is commented-out using `#`. It describes the energy binning that needed to interpret the following data. It can be seen as the head of the following data table. The first column is an integer value describing the simulation time step. The second column counts the number of real particles below the minimum energy value used for the histogram. The following columns give the real electron count of the particles in the specific bin described by the first line/header. The second last column gives the number of real particles that have a higher energy than the maximum energy used for the histogram. The last column gives the total number of particles. In total there are 4 columns more than the number of bins specified with command line arguments. Each row describes another simulation time step.

Analysis Tools

Data Reader

You can quickly load and interact with the data in Python with:

```
from picongpu.plugins.data import EnergyHistogramData

eh_data = EnergyHistogramData('/home/axel/runs/lwfa_001')

# show available iterations
eh_data.get_iterations(species='e')

# show available simulation times
eh_data.get_times(species='e')

# load data for a given iteration
counts, bins_keV, _, _ = eh_data.get(species='e', species_filter='all',␣
↪iteration=2000)

# get data for multiple iterations
counts, bins_keV, iteration, dt = eh_data.get(species='e', iteration=[200, 400,␣
↪8000])

# load data for a given time
counts, bins_keV, iteration, dt = eh_data.get(species='e', species_filter='all',␣
↪time=1.3900e-14)
```

Matplotlib Visualizer

You can quickly plot the data in Python with:

```
from picongpu.plugins.plot_mpl import EnergyHistogramMPL
import matplotlib.pyplot as plt


# create a figure and axes
fig, ax = plt.subplots(1, 1)

# create the visualizer
eh_vis = EnergyHistogramMPL('path/to/run_dir', ax)

eh_vis.visualize(iteration=200, species='e')

plt.show()

# specifying simulation time is also possible (granted there is a matching␣
↪iteration for that time)
eh_vis.visualize(time=2.6410e-13, species='e')

plt.show()

# plotting histogram data for multiple simulations simultaneously also works:
eh_vis = EnergyHistogramMPL([
     ("sim1", "path/to/sim1"),
     ("sim2", "path/to/sim2"),
     ("sim3", "path/to/sim3")], ax)
 eh_vis.visualize(species="e", iteration=10000)

 plt.show()
```

The visualizer can also be used from the command line (for a single simulation only) by writing

```
python energy_histogram_visualizer.py
```

with the following command line options

Options	Value
-p	Path to the run directory of a simulation.
-i	An iteration number
-s (optional, defaults to 'e')	Particle species abbreviation (e.g. 'e' for electrons)
-f (optional, defaults to 'all')	Species filter string

Alternatively, PIConGPU comes with a command line analysis tool for the energy histograms. It is based on *gnuplot* and requires that gnuplot is available via command line. The tool can be found in `src/tools/bin/` and is called `BinEnergyPlot.sh`. It accesses the gnuplot script `BinEnergyPlot.gnuplot` in `src/tools/share/gnuplot/`. `BinEnergyPlot.sh` requires exactly three command line arguments:

Argument	Value
1st	Path and filename to `e_energyHistogram.dat` file.
2nd	Simulation time step (needs to exist)
3rd	Label for particle count used in the graph that this tool produces.

Jupyter Widget

If you want more interactive visualization, then start a jupyter notebook and make sure that `ipywidgets` and `ipympl` are installed.

After starting the notebook server write the following

```
# this is required!
%matplotlib widget
import matplotlib.pyplot as plt
plt.ioff()

from IPython.display import display
from picongpu.plugins.jupyter_widgets import EnergyHistogramWidget

# provide the paths to the simulations you want to be able to choose from
# together with labels that will be used in the plot legends so you still know
# which data belongs to which simulation
w = EnergyHistogramWidget(run_dir_options=[
        ("scan1/sim4", scan1_sim4),
        ("scan1/sim5", scan1_sim5)])
display(w)
```

and then interact with the displayed widgets.

2.4.7 Energy Particles

This plugin computes the **kinetic and total energy summed over all particles** of a species for time steps specified.

.cfg file

Only the time steps at which the total kinetic energy of all particles should be specified needs to be set via command line argument.

PIConGPU command line option	Description
`--e_energy.period 100`	Sets the time step period at which the energy of all **electrons** in the simulation should be simulated. If set to e.g. `100`, the energy is computed for time steps *0, 100, 200, ...*. The default value is `0`, meaning that the plugin does not compute the particle energy.
`--<species>_energy period 42`	Same as above, for any other species available.
`--<species>_energy filter`	Use filtered particles. All available filters will be shown with `picongpu --help`

Memory Complexity

Accelerator

negligible.

Host

negligible.

Output

The plugin creates files prefixed with the species' name and the filter name as postfix, e.g. *e_energy_<filterName>.dat* for the electron energies and *p_energy_<filterName>.dat* for proton energies. The file contains a header describing the columns.

```
#step Ekin_Joule E_Joule
0.0   0.0        0.0
```

Following the header, each line is the output of one time step. The time step is given as first value. The second value is the kinetic energy of all particles at that time step. And the last value is the total energy (kinetic + rest energy) of all particles at that time step.

Attention: The output of this plugin computes a *sum over all particles* in a very naive implementation. This can lead to significant errors due to the finite precision in floating-point numbers. Do not expect the output to be precise to more than a few percent. Do not expect the output to be deterministic due to the statistical nature of the implemented reduce operation.

Please see this issue for a longer discussion and possible future implementations.

Example Visualization

Python snippet:

```
import numpy as np

simDir = "path/to/simOutput/"

# Ekin in Joules (see EnergyParticles)
e_sum_ene = np.loadtxt(simDir + "e_energy_all.dat")[:, 0:2]
p_sum_ene = np.loadtxt(simDir + "p_energy_all.dat")[:, 0:2]
C_sum_ene = np.loadtxt(simDir + "C_energy_all.dat")[:, 0:2]
```

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```
N_sum_ene = np.loadtxt(simDir + "N_energy_all.dat")[:, 0:2]
# Etotal in Joules
fields_sum_ene = np.loadtxt(simDir + "fields_energy.dat")[:, 0:2]

plt.figure()
plt.plot(e_sum_ene[:,0], e_sum_ene[:,1], label="e")
plt.plot(p_sum_ene[:,0], p_sum_ene[:,1], label="p")
plt.plot(C_sum_ene[:,0], C_sum_ene[:,1], label="C")
plt.plot(N_sum_ene[:,0], N_sum_ene[:,1], label="N")
plt.plot(fields_sum_ene[:,0], fields_sum_ene[:,1], label="fields")
plt.plot(
    e_sum_ene[:,0],
    e_sum_ene[:,1] + p_sum_ene[:,1] + C_sum_ene[:,1] + N_sum_ene[:,1] + fields_sum_
↪ene[:,1],
    label="sum"
)
plt.legend()
```

2.4.8 Intensity

The maximum amplitude of the electric field for each cell in y-cell-position in **V/m** and the integrated amplitude of the electric field (integrated over the entire x- and z-extent of the simulated volume and given for each y-cell-position).

Attention: There might be an error in the units of the integrated output.

Note: A renaming of this plugin would be very useful in order to understand its purpose more intuitively.

.cfg file

By setting the PIConGPU command line flag `--intensity.period` to a non-zero value the plugin computes the maximum electric field and the integrated electric field for each cell-wide slice in y-direction. The default value is `0`, meaning that nothing is computed. By setting e.g. `--intensity.period 100` the electric field analysis is computed for time steps *0, 100, 200, ...*

Memory Complexity

Accelerator

negligible.

Host

negligible.

Output

The output of the maximum electric field for each y-slice is stored in `Intensity_max.dat`. The output of the integrated electric field for each y-slice is stored in `Intensity_integrated.dat`.

Both files have two header rows describing the data. .. code:

```
#step position_in_laser_propagation_direction
#step amplitude_data[*]
```

The following odd rows give the time step and then describe the y-position of the slice at which the maximum electric field or integrated electric field is computed. The even rows give the time step again and then the data (maximum electric field or integrated electric field) at the positions given in the previews row.

Known Limitations

- this plugin is only available with the CUDA backend
- this plugin is only available for 3D simulations

Known Issues

Currently, the output file is overwritten after restart. Additionally, this plugin does not work with non-regular domains, see here . This will be fixed in a future version.

There might be an error in the units of the integrated output.

For a full list, see #327 .

2.4.9 ISAAC

This is a plugin for the in-situ library ISAAC [Matthes2016] for a live rendering and steering of PIConGPU simulations.

External Dependencies

The plugin is available as soon as the *ISAAC library* is compiled in.

.cfg file

Command line option	Description
`--isaac.period N`	Sets up, that every *N* th timestep an image will be rendered. This parameter can be changed later with the controlling client.
`--isaac.name NAME`	Sets the *NAME* of the simulation, which is shown at the client.
`--isaac.url URL`	*URL* of the required and running isaac server. Host names and IPs are supported.
`--isaac.port PORT`	*PORT* of the isaac server. The default value is `2458` (for the in-situ plugins), but needs to be changed for tunneling reasons or if more than one server shall run on the very same hardware.
`--isaac.width WIDTH`	Setups the *WIDTH* and *HEIGHT* of the created image(s).
`--isaac.height HEIGHT`	Default is `1024x768`.
`--isaac.direct_pause`	If activated ISAAC will pause directly after the simulation started. Useful for presentations or if you don't want to miss the beginning of the simulation.
`--isaac.quality QUALITY`	Sets the *QUALITY* of the images, which are compressed right after creation. Values between `1` and `100` are possible. The default is `90`, but `70` does also still produce decent results.
`--isaac.timingsFilename NAME`	Enable and write benchmark results into the given file.

The most important settings for ISAAC are `--isaac.period`, `--isaac.name` and `--isaac.url`. A possible addition for your submission `tbg` file could be `--isaac.period 1 --isaac.name ! TBG_jobName --isaac.url YOUR_SERVER`, where the tbg variables `!TBG_jobName` is used as name and `YOUR_SERVER` needs to be set up by yourself.

.param file

The ISAAC Plugin has an *isaac.param*, which specifies which fields and particles are rendered. This can be edited (in your local paramSet), but at runtime also an arbitrary amount of fields (in ISAAC called *sources*) can be deactivated. At default every field and every known species are rendered.

Running and steering a simulation

First of all you need to build and run the isaac server somewhere. On HPC systems, simply start the server on the login or head node since it can be reached by all compute nodes (on which the PIConGPU clients will be running).

Functor Chains

One of the most important features of ISAAC are the **Functor Chains**. As most sources (including fields and species) may not be suited for a direct rendering or even full negative (like the electron density field), the functor chains enable you to change the domain of your field source-wise. A date will be read from the field, the functor chain applied and then **only the x-component** used for the classification and later rendering of the scene. Multiply functors can be applied successive with the Pipe symbol `|`. The possible functors are at default:

- **mul** for a multiplication with a constant value. For vector fields you can choose different value per component, e.g. `mul(1,2,0)`, which will multiply the x-component with 1, the y-component with 2 and the z-component with 0. If less parameters are given than components exists, the last parameter will be used for all components without an own parameter.
- **add** for adding a constant value, which works the same as `mul(...)`.

- **sum** for summarizing all available components. Unlike `mul(...)` and `add(...)` this decreases the dimension of the data to `1`, which is a scalar field. You can exploit this functor to use a different component than the x-component for the classification, e.g. with `mul(0,1,0) | sum`. This will first multiply the x- and z-component with 0, but keep the y-component and then merge this to the x-component.
- **length** for calculating the length of a vector field. Like *sum* this functor reduces the dimension to a scalar field, too. However `mul(0,1,0) | sum` and `mul(0,1,0) | length` do not do the same. As `length` does not know, that the x- and z-component are 0 an expensive square root operation is performed, which is slower than just adding the components up.
- **idem** does nothing, it just returns the input data. This is the default functor chain.

Beside the functor chains the client allows to setup the weights per source (values greater than 6 are more useful for PIConGPU than the default weights of 1), the classification via transfer functions, clipping, camera steering and to switch the render mode to iso surface rendering. Furthermore interpolation can be activated. However this is quite slow and most of the time not needed for non-iso-surface rendering.

Memory Complexity

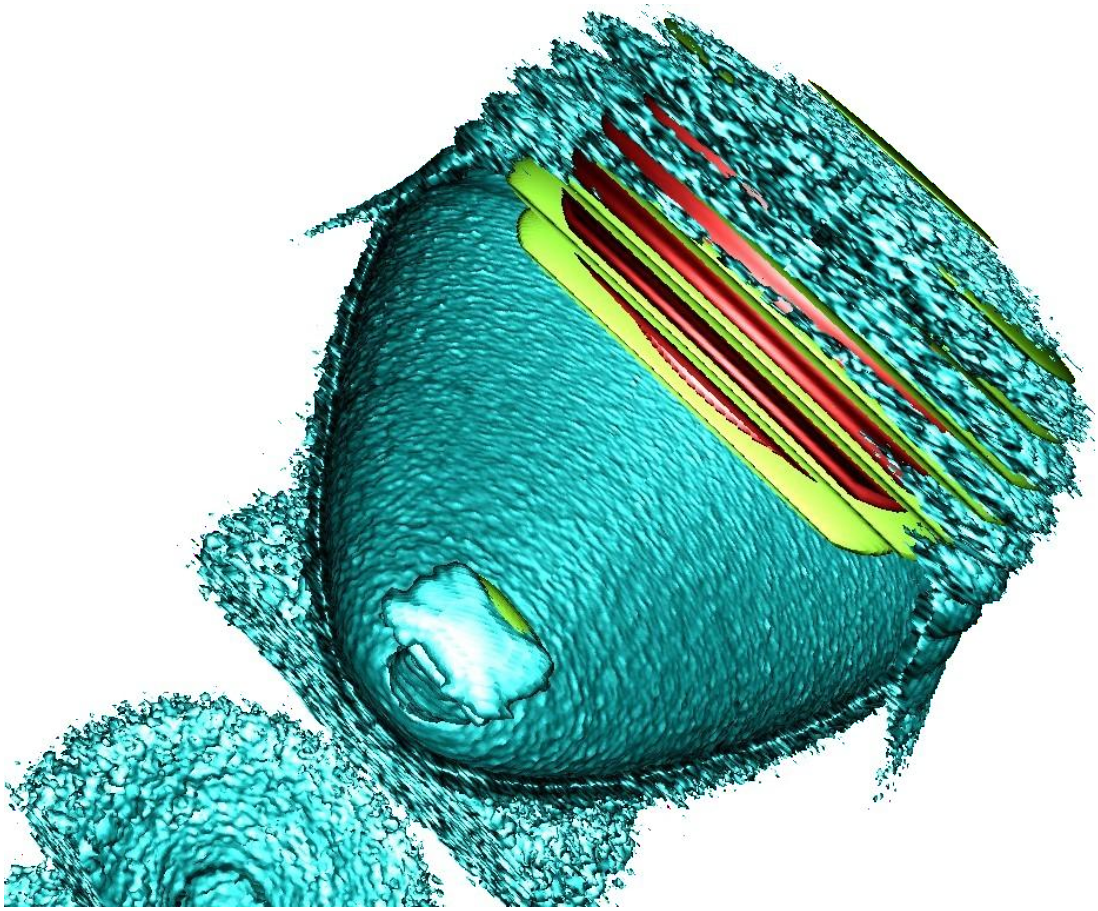
Accelerator

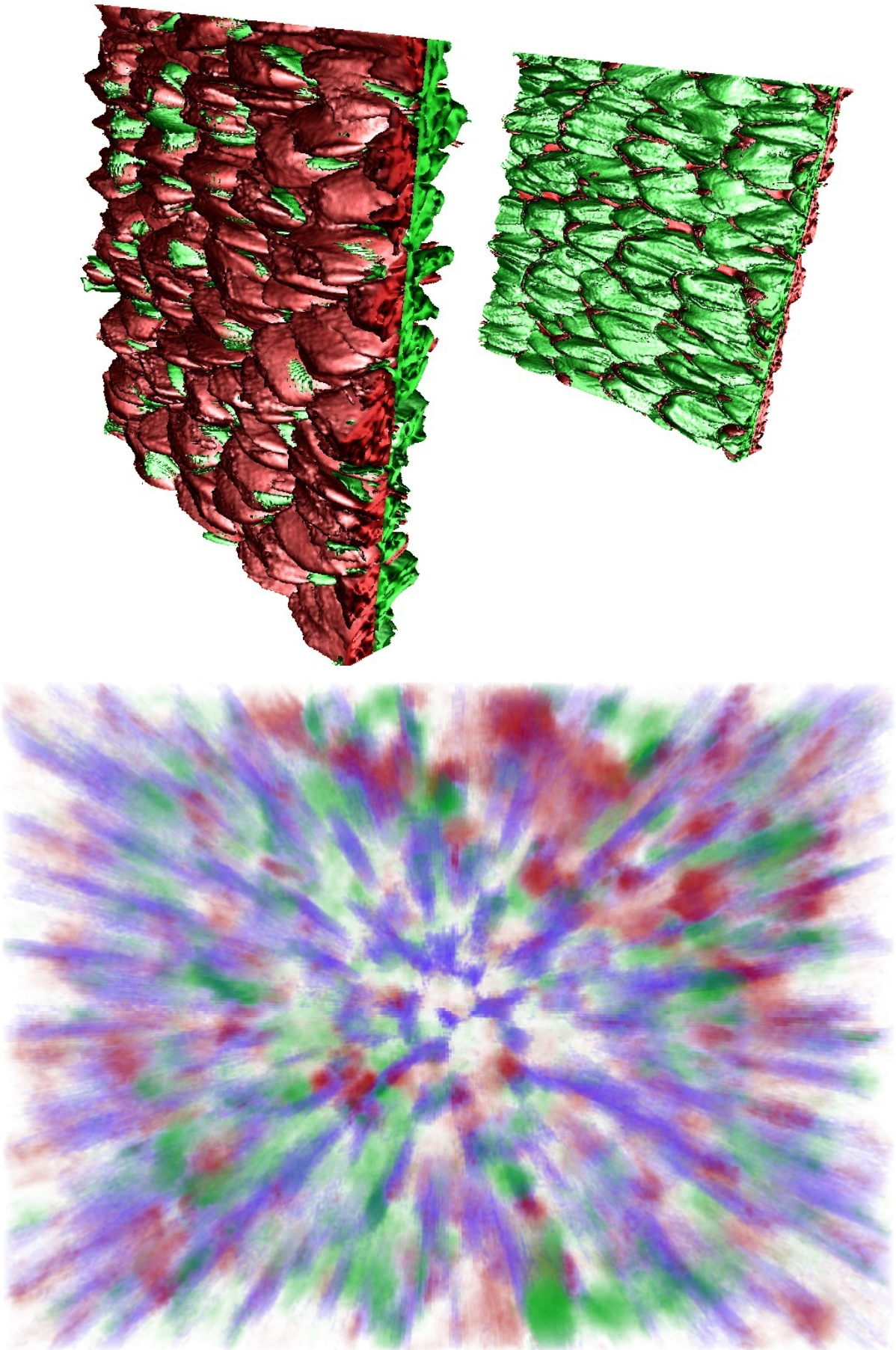
locally, a framebuffer with full resolution and 4 byte per pixel is allocated. For each `FieldTmp` derived field and `FieldJ` a copy is allocated, depending on the input in the *isaac.param* file.

Host

negligible.

Example renderings





References

2.4.10 openPMD

Stores simulation data such as fields and particles according to the openPMD standard using the openPMD API.

External Dependencies

The plugin is available as soon as the *openPMD API* is compiled in. If the openPMD API is found in version 0.13.0 or greater, PIConGPU will support streaming IO via openPMD.

.param file

The corresponding `.param` file is *fileOutput.param*.

One can e.g. disable the output of particles by setting:

```
/* output all species */
using FileOutputParticles = VectorAllSpecies;
/* disable */
using FileOutputParticles = MakeSeq_t< >;
```

Particle filters used for output plugins, including this one, are defined in *particleFilters.param*. Also see *common patterns of defining particle filters*.

.cfg file

You can use `--openPMD.period` to specify the output period. The base filename is specified via `--openPMD.file`. The openPMD API will parse the file name to decide the chosen backend and iteration layout:

- The filename extension will determine the backend.
- The openPMD will either create one file encompassing all iterations (group-based iteration layout) or one file per iteration (file-based iteration layout). The filename will be searched for a pattern describing how to derive a concrete iteration's filename. If no such pattern is found, the group-based iteration layout will be chosen. Please refer to the documentation of the openPMD API for further information.

In order to set defaults for these value, two further options control the filename:

- `--openPMD.ext` sets the filename extension. Possible extensions include `bp` for the ADIOS2 backend (default), `h5` for HDF5 and `sst` for Streaming via ADIOS2/SST. In case your openPMD API supports both ADIOS1 and ADIOS2, make sure that environment variable `OPENPMD_BP_BACKEND` is not set to ADIOS1.
- `--openPMD.infix` sets the filename pattern that controls the iteration layout, default is "_06T" for a six-digit number specifying the iteration. Leave empty to pick group-based iteration layout. Since passing an empty string may be tricky in some workflows, specifying `--openPMD.infix=NULL` is also possible.

  Note that streaming IO requires group-based iteration layout in openPMD, i.e. `--openPMD.infix=NULL` is mandatory. If PIConGPU detects a streaming backend (e.g. by `--openPMD.ext=sst`), it will automatically set `--openPMD.infix=NULL`, overriding the user's choice. Note however that the ADIOS2 backend can also be selected via `--openPMD.json` and via environment variables which PIConGPU does not check. It is hence recommended to set `--openPMD.infix=NULL` explicitly.

Option `--openPMD.source` controls which data is output. Its value is a comma-separated list of combinations of a data set name and a filter name. A user can see all possible combinations for the current setup in the command-line help for this option. Note that addding species and particle filters to `.param` files will automatically extend the number of combinations available. By default all particles and fields are output.

For example, `--openPMD.period 128 --openPMD.file simData --openPMD.source 'species_all'` will write only the particle species data to files of the form `simData_000000.bp`, `simData_000128.bp` in the default simulation output directory every 128 steps. Note that this plugin will only be available if the openPMD API is found during compile configuration.

openPMD backend-specific settings may be controlled via two mechanisms:

- Environment variables. Please refer to the backends' documentations for information on environment variables understood by the backends.
- Backend-specific runtime parameters may be set via JSON in the openPMD API. PIConGPU exposes this via the command line option `--openPMD.json`. Please refer to the openPMD API's documentation for further information.

The JSON parameter may be passed directly as a string, or by filename. The latter case is distinguished by prepending the filename with an at-sign `@`. Specifying a JSON-formatted string from within a `.cfg` file can be tricky due to colliding escape mechanisms. An example for a well-escaped JSON string as part of a `.cfg` file is found below.

```
TBG_openPMD="--openPMD.period 100   \
             --openPMD.file simOutput \
             --openPMD.ext bp \
             --openPMD.json '{ \
                 \"adios2\": { \
                   \"dataset\": { \
                     \"operators\": [ \
                       { \
                         \"type\": \"bzip2\" \
                       } \
                     ] \
                   }, \
                   \"engine\": { \
                     \"type\": \"file\", \
                     \"parameters\": { \
                       \"BufferGrowthFactor\": \"1.2\", \
                       \"InitialBufferSize\": \"2GB\" \
                     } \
                   } \
                 } \
               }'"
```

PIConGPU further defines an **extended format for JSON options** that may alternatively used in order to pass dataset-specific configurations. For each backend `<backend>`, the backend-specific dataset configuration found under `config["<backend>"]["dataset"]` may take the form of a JSON list of patterns: `[<pattern_1>, <pattern_2>, ...]`.

Each such pattern `<pattern_i>` is a JSON object with key `cfg` and optional key `select`: `{"select": <pattern>, "cfg": <cfg>}`.

In here, `<pattern>` is a regex or a list of regexes, as used by POSIX `grep -E`. `<cfg>` is a configuration that will be forwarded as-is to openPMD.

The single patterns will be processed in top-down manner, selecting the first matching pattern found in the list. The regexes will be matched against the openPMD dataset path within the iteration (e.g. `E/x` or `particles/.*/position/.*`), considering full matches only.

The **default configuration** is specified by omitting the `select` key. Specifying more than one default is an error. If no pattern matches a dataset, the default configuration is chosen if specified, or an empty JSON object `{}` otherwise.

A full example:

```
{
  "adios2": {
```

(continues on next page)

(continued from previous page)

```
    "engine": {
      "usesteps": true,
      "parameters": {
        "InitialBufferSize": "2Gb",
        "Profile": "On"
      }
    },
    "dataset": [
      {
        "cfg": {
          "operators": [
            {
              "type": "blosc",
              "parameters": {
                "clevel": "1",
                "doshuffle": "BLOSC_BITSHUFFLE"
              }
            }
          ]
        }
      },
      {
        "select": [
          ".*positionOffset.*",
          ".*particlePatches.*"
        ],
        "cfg": {
          "operators": []
        }
      }
    ]
  }
}
```

Two data preparation strategies are available for downloading particle data off compute devices.

- Set `--openPMD.dataPreparationStrategy doubleBuffer` for use of the strategy that has been optimized for use with ADIOS-based backends. The alias `openPMD.dataPreparationStrategy adios` may be used. This strategy requires at least 2x the GPU main memory on the host side. This is the default.
- Set `--openPMD.dataPreparationStrategy mappedMemory` for use of the strategy that has been optimized for use with HDF5-based backends. This strategy has a small host-side memory footprint (<< GPU main memory). The alias `openPMD.dataPreparationStrategy hdf5` may be used.

PIConGPU command line option	description
`--openPMD.period`	Period after which simulation data should be stored on disk.
`--openPMD.source`	Select data sources and filters to dump. Default is `species_all, fields_all`, which dumps all fields and particle species.
`--openPMD.file`	Relative or absolute openPMD file prefix for simulation data. If relative, files are stored under `simOutput`.
`--openPMD.ext`	openPMD filename extension (this controls thebackend picked by the openPMD API).
`--openPMD.infix`	openPMD filename infix (use to pick file- or group-based layout in openPMD). Set to NULL to keep empty (e.g. to pick group-based iteration layout).
`--openPMD.json`	Set backend-specific parameters for openPMD backends in JSON format.
`--openPMD.dataPreparationStrategy`	Strategy for preparation of particle data (‘doubleBuffer’ or ‘mappedMemory’). Aliases ‘adios’ and ‘hdf5’ may be used respectively.

Note: This plugin is a multi plugin. Command line parameter can be used multiple times to create e.g. dumps with different dumping period. In the case where an optional parameter with a default value is explicitly defined, the parameter will always be passed to the instance of the multi plugin where the parameter is not set. e.g.

```
--openPMD.period 128 --openPMD.file simData1 --openPMD.source 'species_all'
--openPMD.period 1000 --openPMD.file simData2 --openPMD.source 'fields_all' --
↪openPMD.ext h5
```

creates two plugins:

1. dump all species data each 128th time step, use HDF5 backend.
2. dump all field data each 1000th time step, use the default ADIOS backend.

Backend-specific notes

ADIOS2

The memory usage of some engines in ADIOS2 can be reduced by specifying the environment variable `openPMD_USE_STORECHUNK_SPAN=1`. This makes PIConGPU use the span-based Put() API of ADIOS2 which avoids buffer copies, but does not allow for compression. Do *not* use this optimization in combination with compression, otherwise the resulting datasets will not be usable.

Memory Complexity

no extra allocations.

As soon as the openPMD plugin is compiled in, one extra `mallocMC` heap for the particle buffer is permanently reserved. During I/O, particle attributes are allocated one after another. Using `--openPMD.dataPreparationStrategy doubleBuffer` (default) will require at least 2x the GPU memory on the host side. For a smaller host side memory footprint (<< GPU main memory) pick `--openPMD.dataPreparationStrategy mappedMemory`.

Additional Tools

See our *openPMD* chapter.

Experimental: Asynchronous writing

This implements (part of) the workflow described in section 2 of this paper. Rather than writing data to disk directly from PIConGPU, data is streamed via ADIOS2 SST (sustainable streaming transport) to a separate process running asynchronously to PIConGPU. This separate process (`openpmd-pipe`) captures the stream and writes it to disk. `openpmd-pipe` is a Python-based script that comes with recent development versions of openPMD-api (commit bf5174da20e2aeb60ed4c8575da70809d07835ed or newer). A template is provided under `etc/picongpu/summit-ornl/gpu_batch_pipe.tpl` for running such a workflow on the Summit supercompute system. A corresponding single-node runtime configuration is provided for the KelvinHelmholtz example under `share/picongpu/examples/KelvinHelmholtz/etc/picongpu/6_pipe.cfg` (can be scaled up to multi-node). It puts six instances of PIConGPU on one node (one per GPU) and one instance of `openpmd-pipe`.

Advantages:

- Checkpointing and heavy-weight output writing can happen asynchronously, blocking the simulation less.
- Only one file per node is written, implicit node-level aggregation of data from multiple instances of PIConGPU to one instance of `openpmd-pipe` per node. ADIOS2 otherwise also performs explicit node-level data aggregation via MPI; with this setup, ADIOS2 can (and does) skip that step.

- This setup can serve as orientation for the configuration of other loosely-coupled workflows.

Drawbacks:

- Moving all data to another process means that enough memory must be available per node to tolerate that. One way to interpret such a setup is to use idle host memory as a buffer for asynchronous writing in the background.
- Streaming data distribution strategies are not yet mainlined in openPMD-api, meaning that `openpmd-pipe` currently implements a simple ad-hoc data distribution: Data is distributed by simply dividing each dataset into n equal-sized chunks where n is the number of reading processes. In consequence, communication is currently not strictly intra-node. ADIOS2 SST currently relies solely on inter-node communication infrastructure anyway, and performance differences are hence expected to be low.

Notes on the implementation of a proper template file:

- An asynchronous job can be launched by using ordinary Bash syntax for asynchronous launching of processes (`this_is_launched_asynchronously & and_this_is_not;`). Jobs must be waited upon using `wait`.
- Most batch systems will forward all resource allocations of a batch script to launched parallel processes inside the batch script. When launching several processes asynchronously, resources must be allocated explicitly. This includes GPUs, CPU cores and often memory.
- This setup is currently impossible to implement on the HZDR Hemera cluster due to a wrong configuration of the Batch system.

2.4.11 Particle Calorimeter

A binned calorimeter of the amount of kinetic energy per solid angle and energy-per-particle.

The solid angle bin is solely determined by the particle's momentum vector and not by its position, so we are emulating a calorimeter at infinite distance.

The calorimeter takes into account all existing particles as well as optionally all particles which have already left the global simulation volume.

External Dependencies

The plugin is available as soon as the *openPMD API* is compiled in.

.param file

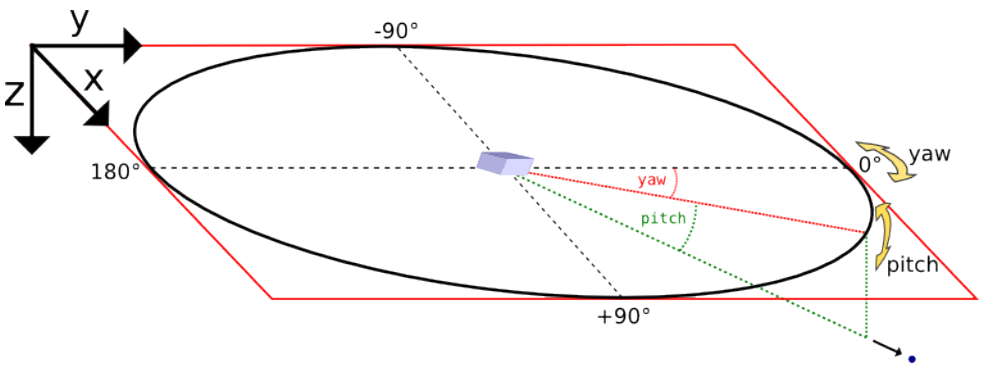
The spatial calorimeter resolution can be customized and in *speciesDefinition.param*. Therein, a species can be also be marked for detecting particles leaving the simulation box.

.cfg file

All options are denoted exemplarily for the photon (`ph`) particle species here.

PIConGPU command line option	Description
`--ph_calorimeter. period`	The ouput periodicity of the plugin. A value of `100` would mean an output at simulation time step *0, 100, 200, ...*
`--ph_calorimeter. file`	Output file suffix. Put unique name if same `species + filter` is used multiple times.
`--ph_calorimeter. ext`	openPMD filename extension. This determines the backend to be used by openPMD. Default is `.h5` for HDF5 output.
`--ph_calorimeter. filter`	Use filtered particles. All available filters will be shown with `picongpu --help`
`--ph_calorimeter. numBinsYaw`	Specifies the number of bins used for the yaw axis of the calorimeter. Defaults to `64`.
`--ph_calorimeter. numBinsPitch`	Specifies the number of bins used for the pitch axis of the calorimeter. Defaults to `64`.
`--ph_calorimeter. numBinsEnergy`	Specifies the number of bins used for the energy axis of the calorimeter. Defaults to `1`, i.e. there is no energy binning.
`--ph_calorimeter. minEnergy`	Minimum detectable energy in keV. Ignored if `numBinsEnergy` is `1`. Defaults to `0`.
`--ph_calorimeter. maxEnergy`	Maximum detectable energy in keV. Ignored if `numBinsEnergy` is `1`. Defaults to `1000`.
`--ph_calorimeter. logScale`	En-/Disable logarithmic energy binning. Allowed values: `0` for disable, `1` enable.
`--ph_calorimeter. openingYaw`	opening angle yaw of the calorimeter in degrees. Defaults to the maximum value: `360`.
`--ph_calorimeter. openingPitch`	opening angle pitch of the calorimeter in degrees. Defaults to the maximum value: `180`.
`--ph_calorimeter. posYaw`	yaw coordinate of the calorimeter position in degrees. Defaults to the +y direction: `0`.
`--ph_calorimeter. posPitch`	pitch coordinate of the calorimeter position in degrees. Defaults to the +y direction: `0`.

Coordinate System



Yaw and pitch are Euler angles defining a point on a sphere's surface, where `(0,0)` points to the `+y` direction here. In the vicinity of `(0,0)`, yaw points to `+x` and pitch to `+z`.

Orientation detail: Since the calorimeters' three-dimensional orientation is given by just two parameters (`posYaw` and `posPitch`) there is one degree of freedom left which has to be fixed. Here, this is achieved by eliminating the Euler angle roll. However, when `posPitch` is exactly `+90` or `-90` degrees, the choice of roll is ambiguous, depending on the yaw angle one approaches the singularity. Here we assume an approach from `yaw = 0`.

Tuning the spatial resolution

By default, the spatial bin size is chosen by dividing the opening angle by the number of bins for yaw and pitch respectively. The bin size can be tuned by customizing the mapping function in `particleCalorimeter.param`.

Memory Complexity

Accelerator

each energy bin times each coordinate bin allocates two counter (`float_X`) permanently and on each accelerator for active and outgoing particles.

Host

as on accelerator.

Output

The calorimeters are stored in hdf5-files in the `simOutput/<species>_calorimeter/<filter>/` directory. The file names are `<species>_calorimeter_<file>_<sfilter>_<timestep>.h5`.

The dataset within the hdf5-file is located at `/data/<timestep>/meshes/calorimeter`. Depending on whether energy binning is enabled the dataset is two or three dimensional. The dataset has the following attributes:

Attribute	Description
`unitSI`	scaling factor for energy in calorimeter bins
`maxYaw[deg]`	half of the opening angle yaw.
`maxPitch[deg]`	half of the opening angle pitch.
`posYaw[deg]`	yaw coordinate of the calorimeter.
`posPitch[deg]`	pitch coordinate of the calorimeter. If energy binning is enabled:
`minEnergy[keV]`	minimal detectable energy.
`maxEnergy[keV]`	maximal detectable energy.
`logScale`	boolean indicating logarithmic scale.

The output in each bin is given in Joule. Divide by energy value of the bin for a unitless count per bin.

The output uses a custom geometry. Since the openPMD API does currently not (yet) support reading from datasets with a custom-name geometry, this plugin leaves the default geometry `"cartesian"` instead of specifying something like `"calorimeter"`. If the output is 2D, cells are defined by *[pitch, yaw]* in degrees. If the output is 3D, cells are defined by *[energy bin, pitch, yaw]* where the energy bin is given in keV. Additionally, if *logScale==1*, then the energy bins are on a logarithmic scale whose start and end can be read from the custom attributes *minEnergy[keV]* and *maxEnergy[keV]* respectively.

Note: This plugin is a multi plugin. Command line parameters can be used multiple times to create e.g. dumps with different dumping period. In the case where an optional parameter with a default value is explicitly defined the parameter will be always passed to the instance of the multi plugin where the parameter is not set. e.g.

```
--ph_calorimeter.period 128 --ph_calorimeter.file calo1 --ph_calorimeter.filter all
--ph_calorimeter.period 1000 --ph_calorimeter.file calo2 --ph_calorimeter.filter␣
↪all --ph_calorimeter.logScale 1 --ph_calorimeter.minEnergy 1
```

creates two plugins:

1. calorimeter for species ph each 128th time step **with** logarithmic energy binning.
2. calorimeter for species ph each 1000th time step **without** (this is the default) logarithmic energy binning.

Attention: When using the plugin multiple times for the same combination of `species` and `filter`, you *must* provide a unique `file` suffix. Otherwise output files will overwrite each other, since only `species`, `filter` and `file` suffix are encoded in it.

An example use case would be two (or more) calorimeters for the same species and filter but with differing position in space or different binning, range, linear and log scaling, etc.

Analysis Tools

The first bin of the energy axis of the calorimeter contains all particle energy less than the minimal detectable energy whereas the last bin contains all particle energy greater than the maximal detectable energy. The inner bins map to the actual energy range of the calorimeter.

Sample script for plotting the spatial distribution and the energy distribution:

```
f = h5.File("<path-to-hdf5-file>")
calorimeter = np.array(f["/data/<timestep>/calorimeter"])

# spatial energy distribution
# sum up the energy spectrum
plt.imshow(np.sum(calorimeter, axis=0))
plt.show()

# energy spectrum
# sum up all solid angles
plt.plot(np.sum(calorimeter, axis=(1,2)))
plt.show()
```

2.4.12 Particle Merger

Merges macro particles that are close in phase space to reduce computational load.

.param file

In *particleMerging.param* is currently one compile-time parameter:

Compile-Time Option	Description
`MAX_VORONOI_CELLS`	Maximum number of active Voronoi cells per supercell. If the number of active Voronoi cells reaches this limit merging events are dropped.

.cfg file

PIConGPU command line option	Description
`--<species>_merger.period`	The ouput periodicity of the plugin. A value of `100` would mean an output at simulation time step *0, 100, 200, ...*.
`--<species>_merger.minParticlesToMerge`	minimal number of macroparticles needed to merge the macroparticle collection into a single macroparticle.
`--<species>_merger.posSpreadThreshold`	Below this threshold of spread in position macroparticles can be merged [unit: cell edge length].
`--<species>_merger.absMomSpreadThreshold`	Below this absolute threshold of spread in momentum macroparticles can be merged [unit: $m_{e^-} \cdot c$]. Disabled for `-1` (default).
`--<species>_merger.relMomSpreadThreshold`	Below this relative (to mean momentum) threshold of spread in momentum macroparticles can be merged [unit: none]. Disabled for `-1` (default).
`--<species>_merger.minMeanEnergy`	minimal mean kinetic energy needed to merge the macroparticle collection into a single macroparticle [unit: keV].

Notes

- `absMomSpreadThreshold` and `relMomSpreadThreshold` are mutually exclusive
- `absMomSpreadThreshold` is always given in [electron mass * speed of light]!

Memory Complexity

Accelerator

no extra allocations, but requires an extra particle attribute per species, `voronoiCellId`.

Host

no extra allocations.

Known Limitations

- this plugin is only available with the CUDA backend
- this plugin might take a significant amount of time due to not being fully parallelized.

Reference

The particle merger implements a macro particle merging algorithm based on:

Luu, P. T., Tueckmantel, T., & Pukhov, A. (2016). Voronoi particle merging algorithm for PIC codes. Computer Physics Communications, 202, 165-174.

There is a slight deviation from the paper in determining the next subdivision. The implementation always tries to subdivide a Voronoi cell by positions first; momentums are only checked in case the spreads in the positions satisfy the threshold.

2.4.13 Particle Merger Probabilistic Version

Merges macro particles that are close in phase space to reduce computational load. Voronoi-based probalistic variative algorithm. The difference between Base Voronoi algorothm and probabilistic version in parameters: instead of threshold of spread in position and momentum use ratio of deleted particles.

.param file

In *particleMerging.param* is currently one compile-time parameter:

Compile-Time Option	Description
`MAX_VORONOI_CELLS`	Maximum number of active Voronoi cells per supercell. If the number of active Voronoi cells reaches this limit merging events are dropped.

.cfg file

PIConGPU command line option	Description
`--<species>_randomizedMerger.period`	The ouput periodicity of the plugin. A value of `100` would mean an output at simulation time step *0, 100, 200, ...*
`--<species>_randomizedMerger.ratioDeletedParticles`	The ratio of particles to delete. The parameter have to be in Range *[0:1]*.
`--<species>_randomizedMerger.maxParticlesToMerge`	Maximum number of macroparticles that can be merged into a single macroparticle.
`--<species>_randomizedMerger.posSpreadThreshold`	Below this threshold of spread in position macroparticles can be merged [unit: cell edge length].
`--<species>_randomizedMerger.momSpreadThreshold`	Below this absolute threshold of spread in momentum macroparticles can be merged [unit: $m_{e^-} \cdot c$].

Memory Complexity

Accelerator

no extra allocations, but requires an extra particle attribute per species, `voronoiCellId`.

Host

no extra allocations.

Known Limitations

- this plugin is only available with the CUDA backend
- this plugin might take a significant amount of time due to not being fully parallelized.

Reference

The particle merger implements a macro particle merging algorithm based on:

Luu, P. T., Tueckmantel, T., & Pukhov, A. (2016). Voronoi particle merging algorithm for PIC codes. Computer Physics Communications, 202, 165-174.

There is a slight deviation from the paper in determining the next subdivision. The implementation always tries to subdivide a Voronoi cell by positions first; momentums are only checked in case the spreads in the positions satisfy the threshold.

2.4.14 Phase Space

This plugin creates a 2D phase space image for a user-given spatial and momentum coordinate.

External Dependencies

The plugin is available as soon as the *openPMD API* is compiled in.

.cfg file

Example for *y-pz* phase space for the *electron* species (`.cfg` file macro):

```
# Calculate a 2D phase space
# - momentum range in m_e c
TGB_ePSypz="--e_phaseSpace.period 10 --e_phaseSpace.filter all --e_phaseSpace.
↪space y --e_phaseSpace.momentum pz --e_phaseSpace.min -1.0 --e_phaseSpace.max 1.
↪0 --e_phaseSpace.ext h5"
```

The distinct options are (assuming a species `e` for electrons):

Option	Usage	Unit
`--e_phaseSpace.period <N>`	calculate each N steps	*none*
`--e_phaseSpace.filter`	Use filtered particles. Available filters are set up in *particleFilters.param*.	*none*
`--e_phaseSpace.space <x/y/z>`	spatial coordinate of the 2D phase space	*none*
`--e_phaseSpace.momentum <px/py/pz>`	momentum coordinate of the 2D phase space	*none*
`--e_phaseSpace.min <ValL>`	minimum of the momentum range	$m_{\text{species}}c$
`--e_phaseSpace.max <ValR>`	maximum of the momentum range	$m_{\text{species}}c$
`--e_phaseSpace.ext <ext>`	filename extension for openPMD backend	*none*

Memory Complexity

Accelerator

locally, a counter matrix of the size local-cells of `space` direction times `1024` (for momentum bins) is permanently allocated.

Host

negligible.

Output

The 2D histograms are stored in the `simOutput/phaseSpace/` directory, by default in `.h5` files. A file is created per species, phasespace selection and time step.

Values are given as *charge density* per phase space bin. In order to scale to a simpler *charge of particles* per $\mathrm{d}r_i$ and $\mathrm{d}p_i$ -bin multiply by the cell volume `dV` (written as an attribute of the openPMD Mesh).

The output writes a number of non-standard custom openPMD attributes:

- `p_min` and `p_max`: The lower and upper bounds for the momentum axis, respectively.
- `dr`: The spacing of the spatial axis in PIConGPU units.
- `dV`: The volume of a phase space cell. Relates to `dr` via `dV = dp * dr` where `dp` would be the grid spacing along the momentum axis.
- `dr_unit`: The SI scaling for the spatial axis. Use this instead of `gridUnitSI`.
- `p_unit`: The SI scaling for the momentum axis. Use this instead of `gridUnitSI`.
- `globalDomainOffset`, `globalDomainSize` and `globalDomainAxisLabels`: Information on the global domain.
- `totalDomainOffset`, `totalDomainSize` and `totalDomainAxisLabels`: Information on the total domain. Please consult the PIConGPU wiki for explanations on the meaning of global and total domain.
- `sim_unit`: SI scaling for the charge density values. Alias for `unitSI`.

Analysis Tools

Data Reader

You can quickly load and interact with the data in Python with:

```
from picongpu.plugins.data import PhaseSpaceData
import numpy as np


ps_data = PhaseSpaceData('/home/axel/runs/lwfa_001')
# show available iterations
ps_data.get_iterations(ps="xpx", species="e", species_filter='all')

# show available simulation times
ps_data.get_times(ps="xpx", species="e", species_filter='all')

# load data for a given iteration
ps, meta = ps_data.get(ps='ypy', species='e', species_filter='all', iteration=2000)

# unit conversion from SI
mu = 1.e6  # meters to microns
e_mc_r = 1. / (9.109e-31 * 2.9979e8)  # electrons: kg * m / s to beta * gamma

Q_dr_dp = np.abs(ps) * meta.dV  # C s kg^-1 m^-2
extent = meta.extent * [mu, mu, e_mc_r, e_mc_r]  # spatial: microns, momentum:␣
↪beta*gamma

# load data for a given time
ps, ps_meta = ps_data.get(ps="xpx", species="e", species_filter='all', time=1.
↪3900e-14)

# load data for multiple iterations
ret = ps_data.get(ps="xpx", species="e", species_filter='all', iteration=[2000,␣
↪4000])

# data and metadata for iteration 2000
# (data is in same order as the value passed to the 'iteration' parameter)
ps, meta = ret[0]
```

Note that the spatial extent of the output over time might change when running a moving window simulation.

Matplotlib Visualizer

You can quickly plot the data in Python with:

```
from picongpu.plugins.plot_mpl import PhaseSpaceMPL
import matplotlib.pyplot as plt


# create a figure and axes
fig, ax = plt.subplots(1, 1)

# create the visualizer
ps_vis = PhaseSpaceMPL('path/to/run_dir', ax)

# plot
ps_vis.visualize(ps="xpx", iteration=200, species='e', species_filter='all')

plt.show()

# specifying simulation time is also possible (granted there is a matching␣
↪iteration for that time)
ps_vis.visualize(ps="xpx", time=2.6410e-13, species='e', species_filter='all')

plt.show()

# plotting data for multiple simulations simultaneously also works:
ps_vis = PhaseSpaceMPL([
     ("sim1", "path/to/sim1"),
     ("sim2", "path/to/sim2"),
     ("sim3", "path/to/sim3")], ax)
ps_vis.visualize(ps="xpx", iteration=10000, species="e", species_filter='all')

plt.show()
```

The visualizer can also be used from the command line (for a single simulation only) by writing

```
python phase_space_visualizer.py
```

with the following command line options

Options	Value
-p	Path and filename to the run directory of a simulation.
-i	An iteration number
-s (optional, defaults to 'e')	Particle species abbreviation (e.g. 'e' for electrons)
-f (optional, defaults to 'all')	Species filter string
-m (optional, defaults to 'ypy')	Momentum string to specify the phase space

Jupyter Widget

If you want more interactive visualization, then start a jupyter notebook and make sure that `ipywidgets` and `ipympl` are installed.

After starting the notebook server write the following

```
# this is required!
%matplotlib widget
import matplotlib.pyplot as plt
plt.ioff()
```

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```
from IPython.display import display
from picongpu.plugins.jupyter_widgets import PhaseSpaceWidget

# provide the paths to the simulations you want to be able to choose from
# together with labels that will be used in the plot legends so you still know
# which data belongs to which simulation
w = PhaseSpaceWidget(run_dir_options=[
        ("scan1/sim4", "/path/to/scan1/sim4"),
        ("scan1/sim5", "/path/to/scan1/sim5")])
display(w)
```

and then interact with the displayed widgets.

Plase note that per default the widget allows selection only of the `ypy` phase space slice for particles labelled by `e`. To visualize, for instance the `ypy`, `xpx` and `ypz` slices for particles labelled by `e` (as a rule background electrons) and by `b` (here electrons of a particle bunch) the above has to be augmented by setting `w.ps.options` and `w.species.options`. The final script snippet then reads:

```
# this is required!
%matplotlib widget
import matplotlib.pyplot as plt
plt.ioff()

from IPython.display import display
from picongpu.plugins.jupyter_widgets import PhaseSpaceWidget

# provide the paths to the simulations you want to be able to choose from
# together with labels that will be used in the plot legends so you still know
# which data belongs to which simulation
w = PhaseSpaceWidget(run_dir_options=[
        ("scan1/sim4", "/path/to/scan1/sim4"),
        ("scan1/sim5", "/path/to/scan1/sim5")])
w.ps.set_trait('options', ('ypy', 'xpx', 'ypz'))
w.species.set_trait('options', ('e', 'b'))
display(w)
```

Out-of-Range Behavior

Particles that are *not* in the range of `<ValL>`/`<ValR>` get automatically mapped to the lowest/highest bin respectively. Take care about that when setting your range and during analysis of the results.

Known Limitations

- only one range per selected space-momentum-pair possible right now (naming collisions)
- charge deposition uses the counter shape for now (would need one more write to neighbors to evaluate it correctly according to the shape)
- the user has to define the momentum range in advance
- the resolution is fixed to `1024 bins` in momentum and the number of cells in the selected spatial dimension
- While the openPMD standard has already been updated to support phase space data, the openPMD API does not yet implement this part. The openPMD attribute `gridUnitSI` and `gridUnitDimension` can hence not be correctly written yet and should be ignored in favor of the custom attributes written by this plugin.

References

The internal algorithm is explained in pull request #347 and in [Huebl2014].

2.4.15 PNG

This plugin generates **images in the png format** for slices through the simulated volume. It allows to draw a **species density** together with electric, magnetic and/or current field values. The exact field values, their coloring and their normalization can be set using `*.param` files. It is a very rudimentary and useful tool to get a first impression on what happens in the simulation and to verify that the parameter set chosen leads to the desired physics.

Note: In the near future, this plugin might be replaced by the ISAAC interactive 3D visualization.

External Dependencies

The plugin is available as soon as the *PNGwriter library* is compiled in.

.cfg file

For **electrons** (`e`) the following table describes the command line arguments used for the visualization.

Command line option	Description
`--e_png.period`	This flag requires an integer value that specifies at what periodicity the png pictures should be created. E.g. setting `--e_png.period 100` generates images for the *0th, 100th, 200th, ...* time step. There is no default. If flags are not set, no pngs are created.
`--e_png.axis`	Set 2D slice through 3D volume that will be drawn. Combine two of the three dimensions `x`, `y``and ``z`, the define a slice. E.g. setting `--e_png.axis yz` draws both the y and z dimension and performs a slice in x-direction.
`--e_png.slicePoint`	Specifies at what ratio of the total depth of the remaining dimension, the slice should be performed. The value given should lie between `0.0` and `1.0`.
`--e_png.folder`	Name of the folder, where all pngs for the above setup should be stored.

These flags use `boost::program_options`'s `multitoken()`. Therefore, **several setups** can be specified e.g. to draw different slices. The order of the flags is important in this case. E.g. in the following example, two different slices are visualized and stored in different directories:

```
picongpu [more args]
  # first
  --e_png.period 100
  --e_png.axis xy
  --e_png.slicePoint 0.5
  --e_png.folder pngElectronsXY
  # second
  --e_png.period 100
  --e_png.axis xz
  --e_png.slicePoint 0.5
  --e_png.folder pngElectronsXZ
```

.param files

The two param files *png.param* and *pngColorScales.param* are used to specify the desired output.

Specifying the field values using `png.param`

Depending on the used prefix in the command line flags, electron and/or ion density is drawn. Additionally to that, three field values can be visualized together with the particle density. In order to set up the visualized field values, the `png.param` needs to be changed. In this file, a variety of other parameters used for the PngModule can be specified.

The ratio of the image can be set.

```
/* scale image before write to file, only scale if value is not 1.0 */
const double scale_image = 1.0;

/* if true image is scaled if cellsize is not quadratic, else no scale */
const bool scale_to_cellsize = true;
```

In order to scale the image, `scale_to_cellsize` needs to be set to `true` and `scale_image` needs to specify the reduction ratio of the image.

Note: For a 2D simulation, even a 2D image can be a quite heavy output. Make sure to reduce the preview size!

It is possible to draw the borders between the GPUs used as white lines. This can be done by setting the parameter `white_box_per_GPU` in `png.param` to `true`

```
const bool white_box_per_GPU = true;
```

There are three field values that can be drawn: `CHANNEL1`, `CHANNEL2` and `CHANNEL3`.

Since an adequate color scaling is essential, there several option the user can choose from.

```
// normalize EM fields to typical laser or plasma quantities
//-1: Auto: enable adaptive scaling for each output
// 1: Laser: typical fields calculated out of the laser amplitude
// 2: Drift: typical fields caused by a drifting plasma
// 3: PlWave: typical fields calculated out of the plasma freq.,
// assuming the wave moves approx. with c
// 4: Thermal: typical fields calculated out of the electron temperature
// 5: BlowOut: typical fields, assuming that a LWFA in the blowout
// regime causes a bubble with radius of approx. the laser's
// beam waist (use for bubble fields)
#define EM_FIELD_SCALE_CHANNEL1 -1
#define EM_FIELD_SCALE_CHANNEL2 -1
#define EM_FIELD_SCALE_CHANNEL3 -1
```

In the above example, all channels are set to **auto scale**. **Be careful**, when using a normalization other than auto-scale, depending on your setup, the normalization might fail due to parameters not set by PIConGPU. *Use the other normalization options only in case of the specified scenarios or if you know, how the scaling is computed.*

You can also add opacity to the particle density and the three field values:

```
// multiply highest undisturbed particle density with factor
float_X const preParticleDens_opacity = 0.25;
float_X const preChannel1_opacity = 1.0;
float_X const preChannel2_opacity = 1.0;
float_X const preChannel3_opacity = 1.0;
```

and add different coloring:

```
// specify color scales for each channel
namespace preParticleDensCol = colorScales::red;   /* draw density in red */
namespace preChannel1Col = colorScales::blue;      /* draw channel 1 in blue */
namespace preChannel2Col = colorScales::green;     /* draw channel 2 in green */
namespace preChannel3Col = colorScales::none;      /* do not draw channel 3 */
```

The colors available are defined in `pngColorScales.param` and their usage is described below. If `colorScales::none` is used, the channel is not drawn.

In order to specify what the three channels represent, three functions can be defined in `png.param`. The define the values computed for the png visualization. The data structures used are those available in PIConGPU.

```
/* png preview settings for each channel */
DINLINE float_X preChannel1( float3_X const & field_B, float3_X const & field_E,␣
↪float3_X const & field_J )
{
    /* Channel1
     * computes the absolute value squared of the electric current */
    return math::abs2(field_J);
}

DINLINE float_X preChannel2( float3_X const & field_B, float3_X const & field_E,␣
↪float3_X const & field_J )
{
    /* Channel2
     * computes the square of the x-component of the electric field */
    return field_E.x() * field_E.x();
}

DINLINE float_X preChannel3( float3_X const & field_B, float3_X const & field_E,␣
↪float3_X const & field_J )
{
    /* Channel3
     * computes the negative values of the y-component of the electric field
     * positive field_E.y() return as negative values and are NOT drawn */
    return -float_X(1.0) * field_E.y();
}
```

Only positive values are drawn. Negative values are clipped to zero. In the above example, this feature is used for `preChannel3`.

Defining coloring schemes in `pngColorScales.param`

There are several predefined color schemes available:

- none (do not draw anything)
- gray
- grayInv
- red
- green
- blue

But the user can also specify his or her own color scheme by defining a namespace with the color name that provides an `addRGB` function:

```
namespace NameOfColor /* name needs to be unique */
{
    HDINLINE void addRGB( float3_X& img, /* the already existing image */
                          const float_X value, /* the value to draw */
                          const float_X opacity ) /* the opacity specified */
```

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```
    {
        /* myChannel specifies the color in RGB values (RedGreenBlue) with
         * each value ranging from 0.0 to 1.0 .
         * In this example, the color yellow (RGB=1,1,0) is used. */
        const float3_X myChannel( 1.0, 1.0, 0.0 );

        /* here, the previously calculated image (in case, other channels have␣
↪already
         * contributed to the png) is changed.
         * First of all, the total image intensity is reduced by the opacity of␣
↪this
         * channel, but only in the color channels specified by this color
↪"NameOfColor".
         * Then, the actual values are added with the correct color (myChannel)␣
↪and opacity. */
        img = img
              - opacity * float3_X( myChannel.x() * img.x(),
                                    myChannel.y() * img.y(),
                                    myChannel.z() * img.z() )
              + myChannel * value * opacity;
    }
}
```

For most cases, using the predefined colors should be enough.

Memory Complexity

Accelerator

locally, memory for the local 2D slice is allocated with 3 channels in `float_X`.

Host

as on accelerator. Additionally, the master rank has to allocate three channels for the full-resolution image. This is the original size **before** reduction via `scale_image`.

Output

The output of this plugin are pngs stored in the directories specified by `--e_png.folder` or `--i_png.folder`. There can be as many of these folders as the user wants. The pngs follow a naming convention:

```
<species>_png_yx_0.5_002000.png
```

First, either `<species>` names the particle type. Following the 2nd underscore, the drawn dimensions are given. Then the slice ratio, specified by `--e_png.slicePoint` or `--i_png.slicePoint`, is stated in the file name. The last part of the file name is a 6 digit number, specifying the simulation time step, at which the picture was created. This naming convention allows to put all pngs in one directory and still be able to identify them correctly if necessary.

Analysis Tools

Data Reader

You can quickly load and interact with the data in Python with:

```
from picongpu.plugins.data import PNGData


png_data = PNGData('path/to/run_dir')

# get the available iterations for which output exists
iters = png_data.get_iterations(species="e", axis="yx")

# get the available simulation times for which output exists
times = png_data.get_times(species="e", axis="yx")

# pngs as numpy arrays for multiple iterations (times would also work)
pngs = png_data.get(species="e", axis="yx", iteration=iters[:3])

for png in pngs:
    print(png.shape)
```

Matplotlib Visualizer

If you are only interested in visualizing the generated png files it is even easier since you don't have to load the data manually.

```
from picongpu.plugins.plot_mpl import PNGMPL
import matplotlib.pyplot as plt


# create a figure and axes
fig, ax = plt.subplots(1, 1)

# create the visualizer
png_vis = PNGMPL('path/to/run_dir', ax)

# plot
png_vis.visualize(iteration=200, species='e', axis='yx')

plt.show()
```

The visualizer can also be used from the command line by writing

```
python png_visualizer.py
```

with the following command line options

Options	Value
-p	Path and to the run directory of a simulation.
-i	An iteration number
-s	Particle species abbreviation (e.g. 'e' for electrons)
-f (optional, defaults to 'e')	Species filter string
-a (optional, defaults to 'yx')	Axis string (e.g. 'yx' or 'xy')
-o (optional, defaults to 'None')	A float between 0 and 1 for slice offset along the third dimension

Jupyter Widget

If you want more interactive visualization, then start a jupyter notebook and make sure that `ipywidgets` and `ipympl` are installed.

After starting the notebook server write the following

```
# this is required!
%matplotlib widget
import matplotlib.pyplot as plt
# deactivate interactive mode
plt.ioff()

from IPython.display import display
from picongpu.plugins.jupyter_widgets import PNGWidget

# provide the paths to the simulations you want to be able to choose from
# together with labels that will be used in the plot legends so you still know
# which data belongs to which simulation
w = PNGWidget(run_dir_options=[
        ("scan1/sim4", scan1_sim4),
        ("scan1/sim5", scan1_sim5)])
display(w)
```

and then interact with the displayed widgets.

2.4.16 Positions Particles

This plugin prints out the *position, momentum, mass, macro particle weighting, electric charge and relativistic gamma factor* of a particle to `stdout` (usually inside the `simOutput/output` file). **It only works with test simulations that have only one particle.**

.cfg file

By setting the command line flag `--<species>_position.period` to a non-zero number, the analyzer is used. In order to get the particle trajectory for each time step the period needs to be set to `1`, meaning e.g. `--e_position.period 1` for electrons. If less output is needed, e.g. only every 10th time step, the period can be set to different values, e.g. `--e_position.period 10`.

Memory Complexity

Accelerator

negligible.

Host

negligible.

Output

The electron trajectory is written directly to the *standard output*. Therefore, it goes both to `simOutput/output` as well as to the output file specified by the machine used (usually the `stdout` file in the main directory of the simulation). The output is ASCII-text only. It has the following format:

```
[ANALYSIS] [MPI_Rank] [COUNTER] [<species>_position] [currentTimeStep] currentTime
↪{position.x position.y position.z} {momentum.x momentum.y momentum.z} mass␣
↪weighting charge gamma
```

Value	Description	Unit
`MPI_Rank`	MPI rank at which prints the particle position	*none*
`COUNTER`	name of the plugin | always `<species>_position`	
`currentTimeStep`	simulation time step = number of PIC cycles	*none*
`currentTime`	simulation time in SI units	seconds
`position.x` `_position.y` `_position.z`	location of the particle in space	meters
`momentum.x` `_momentum.y` `_momentum.z`	momentum of particle	kg m/s
`mass`	mass of macro particle	kg
`weighting`	number of electrons represented by the macro particle	*none*
`charge`	charge of macro particle	Coulomb
`gamma`	relativistic gamma factor of particle	*none*

```
# an example output line:
[ANALYSIS] [2] [COUNTER] [e_position] [878] 1.46440742e-14 {1.032e-05 4.
↪570851689815522e-05 5.2e-06} {0 -1.
337873603181226e-21 0} 9.109382e-31 1 -1.602176e-19 4.999998569488525
```

In order to extract only the trajectory information from the total output stored in `stdout`, the following command on a bash command line could be used:

```
grep "e_position" stdout > trajectory.dat
```

The particle data is then stored in `trajectory.dat`.

In order to extract e.g. the position from this line the following can be used:

```
cat trajectory.dat | awk '{print $7}' | sed -e "s/{//g" | sed -e 's/}//g' | sed -e
↪'s/,/\t/g' > position.dat
```

Known Limitations

- this plugin is only available with the CUDA backend

Known Issues

Attention: This plugin only works correctly if a single particle is simulated. If more than one particle is simulated, the output becomes random, because only the information of one particle is printed. This plugin might be upgraded to work with multiple particles, but better use our openPMD plugin instead and assign `particleIds` to individual particles.

Attention: Currently, both `simOutput/output` and `stdout` are overwritten at restart. All data from the plugin is lost, if these file are not backuped manually.

2.4.17 Radiation

The spectrally resolved far field radiation of charged macro particles.

Our simulation computes the Lienard Wiechert potentials to calculate the emitted electromagnetic spectra for different observation directions using the far field approximation.

$$\frac{\mathrm{d}^2 I}{\mathrm{d}\,\Omega\,\mathrm{d}\,\omega}(\omega, \vec{n}) = \frac{q^2}{16\pi^3 \varepsilon_0 c} \left| \sum_{k=1}^{N} \int_{-\infty}^{+\infty} \frac{\vec{n} \times \left[\left(\vec{n} - \vec{\beta}_k(t) \right) \times \dot{\vec{\beta}}_k(t) \right]}{\left(1 - \vec{\beta}_k(t) \cdot \vec{n} \right)^2} \cdot \mathrm{e}^{\mathrm{i}\,\omega (t - \vec{n} \cdot \vec{r}_k(t)/c)}\,\mathrm{d}\,t \right|^2$$

Details on how radiation is computed with this plugin and how the plugin works can be found in [Pausch2012]. A list of tests can be found in [Pausch2014] and [Pausch2019].

Variable	Meaning
$\vec{r}_k(t)$	The position of particle *k* at time *t*.
$\vec{\beta}_k(t)$	The normalized speed of particle *k* at time *t*. (Speed divided by the speed of light)
$\dot{\vec{\beta}}_k(t)$	The normalized acceleration of particle *k* at time *t*. (Time derivative of the normalized speed.)
t	Time
$\vec{n}$	Unit vector pointing in the direction where the far field radiation is observed.
ω	The circular frequency of the radiation that is observed.
N	Number of all (macro) particles that are used for computing the radiation.
k	Running index of the particles.

Currently this allows to predict the emitted radiation from plasma if it can be described by classical means. Not considered are emissions from ionization, Compton scattering or any bremsstrahlung that originate from scattering on scales smaller than the PIC cell size.

External Dependencies

The plugin is available as soon as the *openPMD API* is compiled in. (Currently it is fixed to use the hdf5 backend until the radiation python module is converted from `h5py` to `openPMD-api`. Therefore, an openPMD API which supports the HDF5 backend is required.)

.param files

In order to setup the radiation analyzer plugin, both the *radiation.param* and the *radiationObserver.param* have to be configured **and** the radiating particles need to have the attribute `momentumPrev1` which can be added in *speciesDefinition.param*.

In *radiation.param*, the number of frequencies `N_omega` and observation directions `N_theta` is defined.

Frequency range

The frequency range is set up by choosing a specific namespace that defines the frequency setup

```
/* choose linear frequency range */
namespace radiation_frequencies = linear_frequencies;
```

Currently you can choose from the following setups for the frequency range:

namespace	Description
`linear_frequencies`	linear frequency range from `SI::omega_min` to `SI::omega_max` with `N_omega` steps
`log_frequencies`	logarithmic frequency range from `SI::omega_min` to `SI::omega_max` with `N_omega` steps
`frequencies_from_list`	`N_omega` frequencies taken from a text file with location `listLocation[]`

All three options require variable definitions in the according namespaces as described below:

For the **linear frequency** scale all definitions need to be in the `picongpu::plugins::radiation::linear_frequencie` namespace. The number of total sample frequencies `N_omega` need to be defined as `constexpr unsigned int`. In the sub-namespace `SI`, a minimal frequency `omega_min` and a maximum frequency `omega_max` need to be defined as `constexpr float_64`.

For the **logarithmic frequency** scale all definitions need to be in the `picongpu::plugins::radiation::log_frequencies` namespace. Equivalently to the linear case, three variables need to be defined: The number of total sample frequencies `N_omega` need to be defined as `constexpr unsigned int`. In the sub-namespace `SI`, a minimal frequency `omega_min` and a maximum frequency `omega_max` need to be defined as `constexpr float_64`.

For the **file-based frequency** definition, all definitions need to be in the `picongpu::plugins::radiation::frequencies_from_list` namespace. The number of total frequencies `N_omega` need to be defined as `constexpr unsigned int` and the path to the file containing the frequency values in units of $[s^{-1}]$ needs to be given as `constexpr const char * listLocation = "/path/to/frequency_list";`. The frequency values in the file can be separated by newlines, spaces, tabs, or any other whitespace. The numbers should be given in such a way, that c++ standard `std::ifstream` can interpret the number e.g., as `2.5344e+16`.

Note: Currently, the variable `listLocation` is required to be defined in the `picongpu::plugins::radiation::frequencies_from_list` namespace, even if `frequencies_from_list` is not used. The string does not need to point to an existing file, as long as the file-based frequency definition is not used.

Observation directions

The number of observation directions `N_theta` is defined in *radiation.param*, but the distribution of observation directions is given in *radiationObserver.param*) There, the function `observation_direction` defines the observation directions.

This function returns the x,y and z component of a **unit vector** pointing in the observation direction.

```
DINLINE vector_64
observation_direction( int const observation_id_extern )
{
    /* use the scalar index const int observation_id_extern to compute an
     * observation direction (x,y,y) */
    return vector_64( x , y , z );
}
```

Note: The `radiationObserver.param` set up will be subject to **further changes**. These might be *namespaces* that describe several preconfigured layouts or a functor if *C++ 11* is included in the *nvcc*.

Nyquist limit

A major limitation of discrete Fourier transform is the limited frequency resolution due to the discrete time steps of the temporal signal. (see Nyquist-Shannon sampling theorem) Due to the consideration of relativistic delays, the sampling of the emitted radiation is not equidistantly sampled. The plugin has the option to ignore any frequency contributions that lies above the frequency resolution given by the Nyquist-Shannon sampling theorem. Because performing this check costs computation time, it can be switched off. This is done via a precompiler pragma:

```
// Nyquist low pass allows only amplitudes for frequencies below Nyquist frequency
// 1 = on (slower and more memory, no Fourier reflections)
// 0 = off (faster but with Fourier reflections)
#define __NYQUISTCHECK__ 0
```

Additionally, the maximally resolvable frequency compared to the Nyquist frequency can be set.

```
namespace radiationNyquist
{
    /* only use frequencies below 1/2*Omega_Nyquist */
    const float NyquistFactor = 0.5;
}
```

This allows to make a save margin to the hard limit of the Nyquist frequency. By using `NyquistFactor = 0.5` for periodic boundary conditions, particles that jump from one border to another and back can still be considered.

Form factor

The *form factor* is a method, which considers the shape of the macro particles when computing the radiation. More details can be found in [Pausch2018] and [Pausch2019].

One can select between different macro particle shapes. Currently eight shapes are implemented. A shape can be selected by choosing one of the available namespaces:

```
/* choosing the 3D CIC-like macro particle shape */
namespace radFormFactor = radFormFactor_CIC_3D;
```

Namespace	Description
`radFormFactor_CIC_3D`	3D Cloud-In-Cell shape
`radFormFactor_TSC_3D`	3D Triangular shaped density cloud
`radFormFactor_PCS_3D`	3D Quadratic spline density shape (Piecewise Cubic Spline assignment function)
`radFormFactor_CIC_1Dy`	Cloud-In-Cell shape in y-direction, dot like in the other directions
`radFormFactor_Gauss_spherical`	symmetric Gauss charge distribution
`radFormFactor_Gauss_cell`	Gauss charge distribution according to cell size
`radFormFactor_incoherent`	forces a completely incoherent emission by scaling the macro particle charge with the square root of the weighting
`radFormFactor_coherent`	forces a completely coherent emission by scaling the macro particle charge with the weighting

Reducing the particle sample

In order to save computation time, only a random subset of all macro particles can be used to compute the emitted radiation. In order to do that, the radiating particle species needs the attribute `radiationMask` (which is initialized as `false`) which further needs to be manipulated, to set to true for specific (random) particles.

Note: The reduction of the total intensity is not considered in the output. The intensity will be (in the incoherent case) will be smaller by the fraction of marked to all particles.

Note: The radiation mask is only added to particles, if not all particles should be considered for radiation calculation. Adding the radiation flag costs memory.

Note: In future updates, the radiation will only be computed using an extra particle species. Therefore, this setup will be subject to further changes.

Gamma filter

In order to consider the radiation only of particles with a gamma higher than a specific threshold, the radiating particle species needs the attribute `radiationMask` (which is initialized as `false`). Using a filter functor as:

```
using RadiationParticleFilter = picongpu::particles::manipulators::FreeImpl<
    GammaFilterFunctor
 >;
```

(see Bunch or Kelvin Helmholtz example for details) sets the flag to true is a particle fulfills the gamma condition.

Note: More sophisticated filters might come in the near future. Therefore, this part of the code might be subject to changes.

Window function filter

A window function can be added to the simulation area to reduce ringing artifacts due to sharp transition from radiating regions to non-radiating regions at the boundaries of the simulation box. This should be applied to simulation setups where the entire volume simulated is radiating (e.g. Kelvin-Helmholtz Instability).

In `radiation.param` the precompiler variable `PIC_RADWINDOWFUNCTION` defines if the window function filter should be used or not.

```
// add a window function weighting to the radiation in order
// to avoid ringing effects from sharp boundaries
// 1 = on (slower but with noise/ringing reduction)
// 0 = off (faster but might contain ringing)
#define PIC_RADWINDOWFUNCTION 0
```

If set to `1`, the window function filter is used.

There are several different window function available:

```
/* Choose different window function in order to get better ringing reduction
 * radWindowFunctionRectangle
 * radWindowFunctionTriangle
 * radWindowFunctionHamming
 * radWindowFunctionTriplett
 * radWindowFunctionGauss
 */
namespace radWindowFunctionRectangle { }
namespace radWindowFunctionTriangle { }
namespace radWindowFunctionHamming { }
namespace radWindowFunctionTriplett { }
namespace radWindowFunctionGauss { }

namespace radWindowFunction = radWindowFunctionTriangle;
```

By setting `radWindowFunction` a specific window function is selected.

More details can be found in [Pausch2019].

.cfg file

For a specific (charged) species `<species>` e.g. `e`, the radiation can be computed by the following commands.

Command line option	Description
`--<species>_radiation period`	Gives the number of time steps between which the radiation should be calculated. Default is `0`, which means that the radiation in never calculated and therefor off. Using `1` calculates the radiation constantly. Any value `>=2` is currently producing nonsense.
`--<species>_radiation dump`	Period, after which the calculated radiation data should be dumped to the file system. Default is `0`, therefor never. In order to store the radiation data, a value `>=1` should be used.
`--<species>_radiation lastRadiation`	If set, the radiation spectra summed between the last and the current dump-time-step are stored. Used for a better evaluation of the temporal evolution of the emitted radiation.
`--<species>_radiation folderLastRad`	Name of the folder, in which the summed spectra for the simulation time between the last dump and the current dump are stored. Default is `lastRad`.
`--<species>_radiation totalRadiation`	If set the spectra summed from simulation start till current time step are stored.
`--<species>_radiation folderTotalRad`	Folder name in which the total radiation spectra, integrated from the beginning of the simulation, are stored. Default `totalRad`.
`--<species>_radiation start`	Time step, at which PIConGPU starts calculating the radiation. Default is `2` in order to get enough history of the particles.
`--<species>_radiation end`	Time step, at which the radiation calculation should end. Default: `0` (stops at end of simulation).
`--<species>_radiation radPerGPU`	If set, each GPU additionally stores its own spectra without summing over the entire simulation area. This allows for a localization of specific spectral features.
`--<species>_radiation folderRadPerGPU`	Name of the folder, where the GPU specific spectra are stored. Default: `radPerGPU`
`--<species>_radiation numJobs`	Number of independent jobs used for the radiation calculation. This option is used to increase the utilization of the device by producing more independent work. This option enables accumulation of data in parallel into multiple temporary arrays, thereby increasing the utilization of the device by increasing the memory footprint Default: `2`

Memory Complexity

Accelerator

locally, `numJobs` times number of frequencies `N_omega` times number of directions `N_theta` is permanently allocated. Each result element (amplitude) is a double precision complex number.

Host

as on accelerator.

Output

Depending on the command line options used, there are different output files.

Command line flag	Output description
`--<species>_totalRadiation`	Contains *ASCII* files that have the total spectral intensity until the timestep specified by the filename. Each row gives data for one observation direction (same order as specified in the `observer.py`). The values for each frequency are separated by *tabs* and have the same order as specified in `radiation.param`. The spectral intensity is stored in the units [Js].
`--<species>_lastRadiation`	has the same format as the output of *totalRadiation*. The spectral intensity is only summed over the last radiation `dump` period.
`--<species>_radPerGPU`	Same output as *totalRadiation* but only summed over each GPU. Because each GPU specifies a spatial region, the origin of radiation signatures can be distinguished.
radiationOpenPMD	In the folder `radiationOpenPMD`, openPMD files (currently hdf5) for each radiation dump and species are stored. These are complex amplitudes in units used by *PIConGPU*. These are for restart purposes and for more complex data analysis.

Text-based output

The text-based output of `lastRadiation` and `totalRadiation` contains the intensity values in SI-units [Js]. Intensity values for different frequencies are separated by spaces, while newlines separate values for different observation directions.

In order to read and plot the text-based radiation data, a python script as follows could be used:

```
import numpy as np
import matplotlib.pyplot as plt
from matplotlib.colors import LogNorm

# frequency definition:
# as defined in the 'radiation.param' file:
N_omega = 1024
omega_min = 0.0 # [1/s]
omega_max = 5.8869e17 # [1/s]
omega = np.linspace(omega_min, omega_max, N_omega)

# observation angle definition:
# as defined in the 'radiation.param' file:
N_observer = 128
# as defined in the 'radiationObserver.param' file:
# this example assumes one used the default Bunch example
# there, the theta values are normalized to the Lorentz factor
theta_min = -1.5 # [rad/gamma]
theta_max = +1.5 # [rad/gamma]
theta = np.linspace(theta_min, theta_max, N_observer)

# load radiation text-based data
rad_data = np.loadtxt('./simOutput/lastRad/e_radiation_2820.dat')

# plot radiation spectrum
plt.figure()
plt.pcolormesh(omega, theta, rad_data, norm=LogNorm())

# add and configure colorbar
cb = plt.colorbar()
cb.set_label(r"$\frac{\mathrm{d}^2 I}{\mathrm{d} \omega \mathrm{d} \Omega} \,␣
↪\mathrm{[Js]}$", fontsize=18)
for i in cb.ax.get_yticklabels():
    i.set_fontsize(14)

# configure x-axis
plt.xlabel(r"$\omega \, \mathrm{[1/s]}$", fontsize=18)
```

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```
plt.xticks(fontsize=14)

# configure y-axis
plt.ylabel(r"$\theta / \gamma$", fontsize=18)
plt.yticks(fontsize=14)

# make plot look nice
plt.tight_layout()
plt.show()
```

openPMD output

The openPMD based data contains the following data structure in `/data/{iteration}/DetectorMesh/` according to the openPMD standard:

Amplitude (Group):

Dataset	Description	Dimensions
`x_Re`	real part, x-component of the complex amplitude	(`N_observer`, `N_omega`, 1)
`x_Im`	imaginary part, x-component of the complex amplitude	(`N_observer`, `N_omega`, 1)
`y_Re`	real part, y-component of the complex amplitude	(`N_observer`, `N_omega`, 1)
`y_Im`	imaginary part, y-component of the complex amplitude	(`N_observer`, `N_omega`, 1)
`z_Re`	real part, z-component of the complex amplitude	(`N_observer`, `N_omega`, 1)
`z_Im`	imaginary part, z-component of the complex amplitude	(`N_observer`, `N_omega`, 1)

Note: Please be aware, that despite the fact, that the SI-unit of each amplitude entry is $[\sqrt{\text{Js}}]$, the stored `unitSI` attribute returns $[\text{Js}]$. This inconsistency will be fixed in the future. Until this inconstincy is resolved, please multiply the datasets with the square root of the `unitSI` attribute to convert the amplitudes to SI units.

DetectorDirection (Group):

Dataset	Description	Dimensions
`x`	x-component of the observation direction $\vec{n}$	(`N_observer`, 1, 1)
`y`	y-component of the observation direction $\vec{n}$	(`N_observer`, 1, 1)
`z`	z-component of the observation direction $\vec{n}$	(`N_observer`, 1, 1)

DetectorFrequency (Group):

Dataset	Description	Dimensions
`omega`	frequency ω of virtual detector bin	(1, `N_omega`, 1)

Please be aware that all datasets in the openPMD output are given in the PIConGPU-intrinsic unit system. In order to convert, for example, the frequencies ω to SI-units one has to multiply with the dataset-attribute *unitSI*.

```
import h5py
f = h5py.File("e_radAmplitudes_2800_0_0_0.h5", "r")
omega_handler = f['/data/2800/DetectorMesh/DetectorFrequency/omega']
omega = omega_handler[0, :, 0] * omega_handler.attrs['unitSI']
f.close()
```

In order to extract the radiation data from the openPMD datasets, PIConGPU provides a python module to read the data and obtain the result in SI-units. An example python script is given below. This currently assumes hdf5 output and will soon become openPMD agnostic.

```
import numpy as np
import matplotlib.pyplot as plt
from matplotlib.colors import LogNorm

from picongpu.plugins.data import RadiationData

# access HDF5 radiation file
radData = RadiationData("./simOutput/radiationHDF5/e_radAmplitudes_2820_0_0_0.h5")

# get frequencies
omega = radData.get_omega()

# get all observation vectors and convert to angle

vec_n = radData.get_vector_n()
gamma = 5.0
theta_norm = np.arctan(vec_n[:, 0]/vec_n[:, 1]) * gamma

# get spectrum over observation angle
spectrum = radData.get_Spectra()

# plot radiation spectrum
plt.figure()
plt.pcolormesh(omega, theta_norm, spectrum, norm=LogNorm())

# add and configure colorbar
cb = plt.colorbar()
cb.set_label(r"$\frac{\mathrm{d}^2 I}{\mathrm{d} \omega \mathrm{d} \Omega} \,␣
↪\mathrm{[Js]}$", fontsize=18)
for i in cb.ax.get_yticklabels():
    i.set_fontsize(14)

# configure x-axis
plt.xlabel(r"$\omega \, \mathrm{[1/s]}$", fontsize=18)
plt.xticks(fontsize=14)

# configure y-axis
plt.ylabel(r"$\theta / \gamma$", fontsize=18)
plt.yticks(fontsize=14)

# make plot look nice
plt.tight_layout()
plt.show()
```

There are various methods besides `get_Spectra()` that are provided by the python module. If a method exists for `_x` (or `_X`) it also exists for `_y` and `_z` (`_Y` and `_Z`) accordingly.

Method	Description
`.get_omega()`	get frequency ω of virtual detector bin in units of $[1/\mathrm{s}]$
`.get_vector_n()`	get observation direction $\vec{n}$
`.get_Spectra()`	get spectrum $\mathrm{d}^2 I/\mathrm{d}\omega\mathrm{d}\Omega$ in units of $[\mathrm{Js}]$
`.get_Polarization_X()`	get spectrum but only for polarization in x-direction
`.get_Amplitude_x()`	get x-component of complex amplitude (unit: $[\sqrt{\mathrm{Js}}]$)
`.get_timestep()`	the iteration (timestep) at which the data was produced (unit: PIC-cycles)

Note: Modules for visualizing radiation data and a widget interface to explore the data interactively will be developed in the future.

Analyzing tools

In `picongp/src/tools/bin`, there are tools to analyze the radiation data after the simulation.

Tool	Description
`plotRadiation`	Reads *ASCII* radiation data and plots spectra over angles as color plots. This is a python script that has its own help. Run `plotRadiation --help` for more information.
`radiationSyntheticDetector`	Reads *ASCII* radiation data and statistically analysis the spectra for a user specified region of observation angles and frequencies. This is a python script that has its own help. Run `radiationSyntheticDetector --help` for more information.
smooth.py	Python module needed by `plotRadiation`.

Known Issues

The plugin supports multiple radiation species but spectra (frequencies and observation directions) are the same for all species.

References

2.4.18 Resource Log

Writes resource information such as rank, position, current simulation step, particle count, and cell count as json or xml formatted string to output streams (file, stdout, stderr).

.cfg file

Run the plugin for each nth time step: `--resourceLog.period n`

The following table will describes the settings for the plugin:

Command line option	Description
`--resourceLog.properties`	Selects properties to write [rank, position, currentStep, particleCount, cellCount]
`--resourceLog.format`	Selects output format [json, jsonpp, xml, xmlpp]
`--resourceLog.stream`	Selects output stream [file, stdout, stderr]
`--resourceLog.prefix`	Selects the prefix for the file stream name

Memory Complexity

Accelerator

no extra allocation.

Host

negligible.

Output / Example

Using the options

```
--resourceLog.period 1 \
--resourceLog.stream stdout \
--resourceLog.properties rank position currentStep particleCount cellCount \
--resourceLog.format jsonpp
```

will write resource objects to stdout such as:

```
[1,1]<stdout>:    "resourceLog": {
[1,1]<stdout>:        "rank": "1",
[1,1]<stdout>:        "position": {
[1,1]<stdout>:            "x": "0",
[1,1]<stdout>:            "y": "1",
[1,1]<stdout>:            "z": "0"
[1,1]<stdout>:        },
[1,1]<stdout>:        "currentStep": "357",
[1,1]<stdout>:        "cellCount": "1048576",
[1,1]<stdout>:        "particleCount": "2180978"
[1,1]<stdout>:    }
[1,1]<stdout>:}
```

For each format there exists always a non pretty print version to simplify further processing:

```
[1,3]<stdout>:{"resourceLog":{"rank":"3","position":{"x":"1","y":"1","z":"0"},
↪"currentStep":"415","cellCount":"1048576","particleCount":"2322324"}}
```

2.4.19 Slice Emittance

The plugin computes the total emittance and the slice emittance (for ten combined cells in the longitudinal direction).

Currently, it outputs only the emittance of the transverse momentum space x-px.

More details on the implementation and tests can be found in the master's thesis [Rudat2019].

External Dependencies

None

.param file

None for now. In the future, adding more compile-time configurations might become necessary (e.g., striding of data output).

.cfg file

All options are denoted for the electron (`e`) particle species here.

PIConGPU command line option	Description
`--e_emittance.period arg`	compute slice emittance [for each n-th step], enable plugin by setting a non-zero value A value of `100` would mean an output at simulation time step *0, 100, 200, . . .* .
`--e_emittance.filter arg`	Use filtered particles. All available filters will be shown with `picongpu --help`

Memory Complexity

Accelerator

Each `x^2`, `p_x^2` and `x * p_x` summation value as well as the number of real electrons `gCount_e` needs to be stored as `float_64` for each y-cell.

Host

as on accelerator (needed for MPI data transfer)

Output

Note: This plugin is a multi plugin. Command line parameters can be used multiple times to create e.g. dumps with different dumping period. In the case where an optional parameter with a default value is explicitly defined the parameter will be always passed to the instance of the multi plugin where the parameter is not set. e.g.

```
--e_emittance.period 1000 --e_emittance.filter all
--e_emittance.period  100 --e_emittance.filter highEnergy
```

creates two plugins:

1. slice emittance for species e each 1000th time step for **all** particles.
2. slice emittance for species e each 100th time step **only for particles** with high energy (defined by filter).

Analysis Tools

The output is a text file with the first line as a comment describing the content. The first column is the time step. The second column is the total emittance (of all particles defined by the filter). Each following column is the emittance if the slice at ten cells around the position given in the comment line.

```
data = np.loadtxt("<path-to-emittance-file>")
timesteps = data[:, 0]
total_emittance = data[:, 1]
slice_emittance = data[:, 2:]

# time evolution of total emitance
plt.plot(timesteps, total_emittance)
plt.xlabel("time step")
plt.ylabel("emittance")
plt.show()

# plot slice emittance over time and longitudinal (y) position
plt.imshow(slice_emittance)
plt.xlabel("y position [arb.u.]")
plt.ylabel("time [arb.u.]")
cb = plt.colorbar()
cb.set_label("emittance")
plt.show()
```

References

2.4.20 Slice Field Printer

Outputs a 2D slice of the **electric, magnetic and/or current field** in SI units. The slice position and the field can be specified by the user.

.cfg file

The plugin works on **electric**, **magnetic**, and **current** fields. For the electric field, the prefix `--E_slice.` for all command line arguments is used. For the magnetic field, the prefix `--B_slice.` is used. For the current field, the prefix `--J_slice.` is used.

The following table will describe the setup for the electric field. The same applied to the magnetic field. Only the prefix has to be adjusted.

Command line option	Description
`--E_slice.period`	The periodicity of the slice print out. If set to a non-zero value, e.g. to `--E_slice.period 100`, the slices are generated for every 100th simulation time step.
`--E_slice.fileName`	Name of the output file. Setting *–E_slice.fileName myName* will result in output files like `myName_100.dat`.
`--E_slice.plane`	Defines the plane that the slice will be parallel to. The plane is defined by its orthogonal axis. By using `0` for the x-axis, `1` for the y-axis and `2` for the z-axis, all standard planes can be selected. E.g. choosing the x-y-plane is done by setting the orthogonal axis to the z-axis by giving the command line argument `--E_slice.plane 2`.
`--E_slice.slicePoint`	Defines the position of the slice on the orthogonal axis. E.g. when the x-y-plane was selected, the slice position in z-direction has to be set. This is done using a value between `0.0` and `1.0`. E.g. by setting `--E_slice.slicePoint 0.5`, the slice is centered.

This plugin **supports using multiple slices**. By setting the command line arguments multiple times, multiple slices are printed to file. As an example, the following command line will create two slices:

```
picongpu # [...]
  --E_slice.period 100 --E_slice.fileName slice1 --E_slice.plane 2 --E_slice.
↪slicePoint 0.5
  --E_slice.period  50 --E_slice.fileName slice2 --E_slice.plane 0 --E_slice.
↪slicePoint 0.25
```

The first slice is a cut along the x-y axis. It is printed every 100th step. It cuts through the middle of the z-axis and the data is stored in files like *slice1_100.dat*. The second slice is a cut along the y-z axis. It is printed every 50th step. It cuts through the first quarter of the x-axis and the data is stored in files like *slice2_100.dat*.

2D fields

In the case of 2D fields, the plugin outputs a 1D slice. Be aware that `--E_slice.plane` still refers to the orthogonal axis, i.e. `--E_slice.plane 1` outputs a line along the **x-axis** and `--E_slice.plane 0` along the **y-axis**.

Memory Complexity

Accelerator

the local slice is permanently allocated in the type of the field (`float3_X`).

Host

as on accelerator.

Output

The output is stored in an ASCII file for every time step selected by `.period` (see *How to set it up?*). The 2D slice is stored as lines and rows of the ASCII file. Spaces separate rows and newlines separate lines. Each entry is of the format `{1.1e-1,2.2e-2,3.3e.3}` giving each value of the vector field separately e.g. `{E_x,E_y,E_z}`.

In order to read this data format, there is a python module in `lib/python/picongpu/plugins/sliceFieldReader.py`. The function `readFieldSlices` needs a data file (file or filename) with data from the plugin and returns the data as numpy-array of size `(N_y, N_x, 3)`

Known Limitations

- this plugin is only available with the CUDA backend

Known Issues

See issue #348.

Should be solved with pull request #548.

2.4.21 Sum Currents

This plugin computes the total current integrated/added over the entire volume simulated.

.cfg file

The plugin can be activated by setting a non-zero value with the command line flag `--sumcurr.period`. The value set with `--sumcurr.period` is the periodicity, at which the total current is computed. E.g. `--sumcurr.period 100` computes and prints the total current for time step *0, 100, 200, . . .* .

Memory Complexity

Accelerator

negligible.

Host

negligible.

Output

The result is printed to *standard output*. Therefore, it goes both to `./simOutput/output` as well as to the output file specified by the machine used (usually the `stdout` file in the main directory of the simulation). The output is ASCII-text only. It has the following format:

```
[ANALYSIS] [_rank] [COUNTER] [SumCurrents] [_currentTimeStep] {_current.x _current.
↪y _current.z} Abs:_absCurrent
```

Value	Description	Unit
`_rank`	MPI rank at which prints the particle position	*none*
`_currentTimeStep`	simulation time step = number of PIC cycles	*none*
`_current.x` `_current.y` `_current.z`	electric current	Ampere per second
`_absCurrent`	magnitude of current	Ampere per second

In order to extract only the total current information from the output stored in *stdout*, the following command on a bash command line could be used:

```
grep SumCurrents stdout > totalCurrent.dat
```

The plugin data is then stored in `totalCurrent.dat`.

Known Limitations

- this plugin is only available with the CUDA backend

Known Issues

Currently, both `output` and `stdout` are overwritten at restart. All data from the plugin is lost, if these file are not backuped manually.

2.4.22 Transition Radiation

The spectrally resolved far field radiation created by electrons passing through a metal foil.

Our simulation computes the transition radiation to calculate the emitted electromagnetic spectra for different observation angles.

$$\frac{d^2W}{d\omega d\Omega} = \frac{e^2 N_e}{(4\pi\epsilon_0)\pi^2 c}\left\{\left[\int d^3\vec{p} g(\mathcal{E}_\parallel^2 + \mathcal{E}_\perp^2)\right] + (N_e - 1)\left[\left|\int d^3\vec{p} g \mathcal{E}_\parallel F\right|^2 + \left|\int d^3\vec{p} g \mathcal{E}_\perp F\right|^2\right]\right\}$$

$$\mathcal{E}_\parallel = \frac{u\cos\psi\left[u\sin\psi\cos\phi - (1+u^2)^{1/2}\sin\theta\right]}{\mathcal{N}(\theta,u,\psi,\phi)}$$

$$\mathcal{E}_\perp = \frac{u^2\cos\psi\sin\psi\sin\phi\cos\theta}{\mathcal{N}(\theta,u,\psi,\phi)}$$

$$\mathcal{N}(\theta,u,\psi,\phi) = \left[\left(1+u^2\right)^{1/2} - u\sin\psi\cos\phi\sin\theta\right]^2 - u^2\cos^2\psi\cos^2\theta$$

$$F = \frac{1}{g(\vec{p})}\int d^2\vec{r}_\perp e^{-i\vec{k}_\perp\cdot\vec{r}_\perp}\int dy e^{-iy(\omega - \vec{k}_\perp\cdot\vec{v}_\perp)/v_y} h(\vec{r},\vec{p})$$

Variable	Meaning
N_e	Amount of real electrons
ψ	Azimuth angle of momentum vector from electrons to y-axis of simulation
θ	Azimuth angle of observation vector
ϕ	Polar angle between momentum vector from electrons and observation vector
ω	The circular frequency of the radiation that is observed.
$h(\vec{r}, \vec{p})$	Normalized phasespace distribution of electrons
$g(\vec{p})$	Normalized momentum distribution of electrons
$g(\vec{p})$	Normalized momentum distribution of electrons
$\vec{k}$	Wavevector of electrons
$\vec{v}$	Velocity vector of electrons
u	Normalized momentum of electrons $\beta\gamma$
$\mathcal{E}$	Normalized energy of electrons
$\mathcal{N}$	Denominator of normalized energies
F	Normalized formfactor of electrons, contains phase informations

This plugin allows to predict the emitted virtual transition radiation, which would be caused by the electrons in the simulation box passing through a virtual metal foil which is set at a specific location. The transition radiation can only be calculated for electrons at the moment.

External Dependencies

There are no external dependencies.

.param files

In order to setup the transition radiation plugin, the *transitionRadiation.param* has to be configured **and** the radiating particles need to have the attributes `weighting`, `momentum`, `location`, and `transitionRadiationMask` (which can be added in *speciesDefinition.param*) as well as the flags `massRatio` and `chargeRatio`.

In *transitionRadiation.param*, the number of frequencies `N_omega` and observation directions `N_theta` and `N_phi` are defined.

Frequency range

The frequency range is set up by choosing a specific namespace that defines the frequency setup

```
/* choose linear frequency range */
namespace radiation_frequencies = linear_frequencies;
```

Currently you can choose from the following setups for the frequency range:

namespace	Description
`linear_frequencies`	linear frequency range from `SI::omega_min` to `SI::omega_max` with `N_omega` steps
`log_frequencies`	logarithmic frequency range from `SI::omega_min` to `SI::omega_max` with `N_omega` steps
`frequencies_from_list`	`N_omega` frequencies taken from a text file with location `listLocation[]`

All three options require variable definitions in the according namespaces as described below:

For the **linear frequency** scale all definitions need to be in the `picongpu::plugins::transitionRadiation::linear_` namespace. The number of total sample frequencies `N_omega` need to be defined as `constexpr unsigned`

`int`. In the sub-namespace `SI`, a minimal frequency `omega_min` and a maximum frequency `omega_max` need to be defined as `constexpr float_64`.

For the **logarithmic frequency** scale all definitions need to be in the `picongpu::plugins::transitionRadiation::log_frequencies` namespace. Equivalently to the linear case, three variables need to be defined: The number of total sample frequencies `N_omega` need to be defined as `constexpr unsigned int`. In the sub-namespace `SI`, a minimal frequency `omega_min` and a maximum frequency `omega_max` need to be defined as `constexpr float_64`.

For the **file-based frequency** definition, all definitions need to be in the `picongpu::plugins::transitionRadiation::frequencies_from_list` namespace. The number of total frequencies `N_omega` need to be defined as `constexpr unsigned int` and the path to the file containing the frequency values in units of $[s^{-1}]$ needs to be given as `constexpr const char * listLocation = "/path/to/frequency_list";`. The frequency values in the file can be separated by newlines, spaces, tabs, or any other whitespace. The numbers should be given in such a way, that c++ standard `std::ifstream` can interpret the number e.g., as `2.5344e+16`.

Note: Currently, the variable `listLocation` is required to be defined in the `picongpu::plugins::transitionRadiation::frequencies_from_list` namespace, even if `frequencies_from_list` is not used. The string does not need to point to an existing file, as long as the file-based frequency definition is not used.

Observation directions

The number of observation directions `N_theta` and the distribution of observation directions is defined in *transitionRadiation.param*. There, the function `observation_direction` defines the observation directions.

This function returns the x,y and z component of a **unit vector** pointing in the observation direction.

```
DINLINE vector_64
observation_direction( int const observation_id_extern )
{
    /* use the scalar index const int observation_id_extern to compute an
     * observation direction (x,y,y) */
    return vector_64( x , y , z );
}
```

Note: The `transitionRadiation.param` set up will be subject to **further changes**, since the `radiationObserver.param` it is based on is subject to further changes. These might be *namespaces* that describe several preconfigured layouts or a functor if *C++ 11* is included in the *nvcc*.

Foil Position

If one wants to virtually propagate the electron bunch to a foil in a further distance to get a rough estimate of the effect of the divergence on the electron bunch, one can include a foil position. A foil position which is unequal to zero, adds the electrons momentum vectors onto the electron until they reach the given y-coordinate. To contain the longitudinal information of the bunch, the simulation window is actually virtually moved to the foil position and not each single electron.

```
namespace SI
{
    // y position of the foil to calculate transition radiation at
    // leave at 0 for no virtual particle propagation
    constexpr float_64 foilPosition = 0.0;
}
```

Note: This is an experimental feature, which was not verified yet.

Macro-particle form factor

The *macro-particle form factor* is a method, which considers the shape of the macro particles when computing the radiation.

One can select between different macro particle shapes. Currently eight shapes are implemented. A shape can be selected by choosing one of the available namespaces:

```
/* choosing the 3D CIC-like macro particle shape */
namespace radFormFactor = radFormFactor_CIC_3D;
```

Namespace	Description
`radFormFactor_CIC_3D`	3D Cloud-In-Cell shape
`radFormFactor_TSC_3D`	3D Triangular shaped density cloud
`radFormFactor_PCS_3D`	3D Quadratic spline density shape (Piecewise Cubic Spline assignment function)
`radFormFactor_CIC_1Dy`	Cloud-In-Cell shape in y-direction, dot like in the other directions
`radFormFactor_Gauss_spherical`	symmetric Gauss charge distribution
`radFormFactor_Gauss_cell`	Gauss charge distribution according to cell size
`radFormFactor_incoherent`	forces a completely incoherent emission by scaling the macro particle charge with the square root of the weighting
`radFormFactor_coherent`	forces a completely coherent emission by scaling the macro particle charge with the weighting

Note: One should not confuse this macro-particle form factor with the form factor F, which was previously mentioned. This form factor is equal to the macro-particle shape, while F contains the phase information of the whole electron bunch. Both are necessary for a physically correct transition radiation calculation.

Gamma filter

In order to consider the radiation only of particles with a gamma higher than a specific threshold. In order to do that, the radiating particle species needs the flag `transitionRadiationMask` (which is initialized as `false`) which further needs to be manipulated, to set to true for specific (random) particles.

Using a filter functor as:

```
using GammaFilter = picongpu::particles::manipulators::generic::Free<
    GammaFilterFunctor
>;
```

(see TransitionRadiation example for details) sets the flag to true if a particle fulfills the gamma condition.

Note: More sophisticated filters might come in the near future. Therefore, this part of the code might be subject to changes.

.cfg file

For a specific (charged) species `<species>` e.g. `e`, the radiation can be computed by the following commands.

Command line option	Description
`--<species>_transRad.period`	Gives the number of time steps between which the radiation should be calculated.

Memory Complexity

Accelerator

two counters (`float_X`) and two counters (`complex_X`) are allocated permanently

Host

as on accelerator.

Output

Contains *ASCII* files in `simOutput/transRad` that have the total spectral intensity until the timestep specified by the filename. Each row gives data for one observation direction (same order as specified in the `observer.py`). The values for each frequency are separated by *tabs* and have the same order as specified in `transitionRadiation.param`. The spectral intensity is stored in the units **[J s]**.

Analysing tools

The `transition_radiation_visualizer.py` in `lib/python/picongpu/plugins/plot_mpl` can be used to analyze the radiation data after the simulation. See `transition-radiation_visualizer.py --help` for more information. It only works, if the input frequency are on a divided logarithmically!

Known Issues

The output is currently only physically correct for electron passing through a metal foil.

References

- ***Theory of coherent transition radiation generated at a plasma-vacuum interface*** Schroeder, C. B. and Esarey, E. and van Tilborg, J. and Leemans, W. P., American Physical Society(2004), https://link.aps.org/doi/10.1103/PhysRevE.69.016501
- ***Diagnostics for plasma-based electron accelerators*** Downer, M. C. and Zgadzaj, R. and Debus, A. and Schramm, U. and Kaluza, M. C., American Physical Society(2018), https://link.aps.org/doi/10.1103/RevModPhys.90.035002
- ***Synthetic characterization of ultrashort electron bunches using transition radiation*** Carstens, F.-O., Bachelor thesis on the transition radiation plugin, https://doi.org/10.5281/zenodo.3469663
- ***Quantitatively consistent computation of coherent and incoherent radiation in particle-in-cell codes — A general form fac*** Pausch, R., Description for the effect of macro-particle shapes in particle-in-cell codes, https://doi.org/10.1016/j.nima.2018.02.020

2.4.23 xrayScattering

This plugin calculates Small Angle X-ray Scattering (SAXS) patterns from electron density. (Using a density *FieldTmp* as an intermediate step and not directly the macro particle distribution.) This is a species specific plugin and it has to be run separately for each scattering species. Since the plugin output is the scattered complex amplitude, contributions from different species can be coherently summed later on.

$$\Phi(\vec{q}) = \frac{r_e}{d} \int_t \mathrm{d}t \int_V \mathrm{d}V \phi(\vec{r}, t) n(\vec{r}, t)$$
$$I = |\Phi|^2$$

Variable	Meaning
Φ	Scattered amplitude
$\vec{q}$	Scattering vector with $\lvert\vec{q}\rvert = \frac{4\pi \sin\theta}{\lambda}$
θ	Scattering angle. 2θ is the angle between the incoming and the scattered k-vectors.
λ	Probing beam wavelength
n	Electron density
ϕ	Incoming wave amplitude
I	Scattering intensity
d	Screen distance
r_e	Classical electron radius

For the free electrons, the density n is just their number density, for ions it is the bound electrons density of the species. This plugin will automatically switch to bound electrons density for species having the *boundElectrons* property.

The volume integral is realized by a discrete sum over the simulation cells and the temporal integration reduces to accumulating the amplitude over simulation time steps.

Note: This calculation is based on the kinematic model of scattering. Multiple scattering CAN NOT be handled in this model.

External Dependencies

The plugin is available as soon as the *openPMD API* is compiled in.

.param file

The *xrayScattering.param* file sets the x-ray beam alignment as well as its temporal and transverse envelope.

Note: At the moment the translation (to the side center + offset) is not working correctly. For that reason, the envelopes and the offset can't be set in the `.param` file yet. The probe is always a plane wave. Beam rotation works.

The alignment settings define a beam coordinate system with $\hat{z} = \hat{k}$ and $\hat{x}, \hat{y}$ perpendicular to the x-ray propagation direction. It is always a right-hand system. It is oriented in such way that for propagation parallel to the PIC x- or y-axis (*Side*: *X*, *XR*, *Y* or *YR*) $\hat{x}_{\text{beam}} = -\hat{z}_{\text{PIC}}$ holds and if $\vec{k}$ is parallel to the PIC z-axis (*Side*: *Z* or *ZR*), $\hat{x}_{\text{beam}} = -\hat{y}_{\text{PIC}}$ holds. The orientation can be then fine adjusted with the *RotationParam* setting. .. TODO: Figures showing the beam coordinate system orientation in the PIC system.

Setting	Description
`ProbingSide`	The side from which the x-ray is propagated. Set *X*, *Y* or *Z* for propagation along one of the PIC coordinate system axes; *XR*, *YR* or *ZR* for propagation in an opposite direction.
`RotationParam`	Rotation of the beam axis, z_{beam}, from the default orientation (perpendicular the the simulation box side). Set the beam yaw and pitch angles in radians.

The coordinate transfer from the PIC system to the beam system is performed in the following order: rotation to one of the default orientations (`ProbingSide` setting), additional rotation (`RotationParam`). This has to be taken into account when defining the experimental setup.

.cfg file

For a specific (charged) species `<species>` e.g. `e`, the scattering can be computed by the following commands.

Command line option	Description
`--<species>_xrayScattering period`	Period at which the plugin is enabled (PIC period syntax). Only the intensity from this steps is accumulated. Default is *0*, which means that the scattering intensity in never calculated and therefor off
`--<species>_xrayScattering outputPeriod`	Period at which the accumulated amplitude is written to the output file (PIC period syntax). Usually set close to the x-ray coherence time.
`--<species>_xrayScattering qx_max`	Upper bound of reciprocal space range in qx direction. The unit is $^{-1}$. Default is *5*.
`--<species>_xrayScattering qy_max`	Upper bound of reciprocal space range in qy direction. The unit is $^{-1}$ Default is *5*.
`--<species>_xrayScattering qx_min`	Lower bound of reciprocal space range in qx direction. The unit is $^{-1}$ Default is *-5*.
`--<species>_xrayScattering qy_min`	Lower bound of reciprocal space range in qy direction. The unit is $^{-1}$ Default is *-5*.
`--<species>_xrayScattering n_qx`	Number of scattering vectors needed to be calculated in qx direction. Default is *100*,
`--<species>_xrayScattering n_qy`	Number of scattering vectors needed to be calculated in qy direction. Default is '100'.
`--<species>_xrayScattering file`	Output file name. Default is *<species>_xrayScatteringOutput*.
`--<species>_xrayScattering ext`	*openPMD* filename extension. This controls the backend picked by the *openPMD* API. Default is *bp* for adios2 backend.
`--<species>_xrayScattering memoryLayout`	Possible values: *mirror* and *split*. Output can be mirrored on all Host+Device pairs or uniformly split, in chunks, over all nodes. Use split when the output array is too big to store the complete computed q-space on one device. For small output grids the *mirror* setting could turn out to be more efficient.

Output

`<species>_xrayScatteringOutput.<backend-specific extension>`

Output file in the *openPMD* standard. An example on how to access your data with the python reader:

```
from picongpu.plugins.data import XrayScatteringData

simulation_path = '...' # dir containing simOutput, input, ..,
# Read output from the 0th step, for electrons, hdf5 backend.
data = XrayScatteringData( simulation_path, 'e', 'h5' )
amplitude = saxsData.get(iteration=0) * saxsData.get_unit()
del XrayScatteringData
```

When you don't want to use the python reader keep in mind that:

- All iterations are saved in a single file
- The mesh containing the output is called *'amplitude'*
- This mesh has 2 components, *'x'* is the real part and *'y'* is the imaginary part.

Note: The amplitude is not zeroed on `outputPeriod` so one has to subtract the output from the iteration one period before and then calculate $|\Phi|^2$ and sum it with the intensities from other coherence periods.

References

- [1] Kluge, T., Rödel, C., Rödel, M., Pelka, A., McBride, E. E., Fletcher, L. B., ... Cowan, T. E. (2017). Nanometer-scale characterization of laser-driven compression, shocks, and phase transitions, by x-ray scattering using free electron lasers. Physics of Plasmas, 24(10). https://doi.org/10.1063/1.5008289

2.4.24 Period Syntax

Most plugins allow to define a period on how often a plugin shall be executed (notified). Its simple syntax is: `<period>` with a simple number.

Additionally, the following syntax allows to define intervals for periods:

`<start>:<end>[:<period>]`

- <*start*>: begin of the interval; default: 0
- <*end*>: end of the interval, including the upper bound; default: end of the simulation
- <*period*>: notify period within the interval; default: 1

Multiple intervals can be combined via a comma separated list.

Examples

- `42` every 42th time step
- `::` equal to just writing `1`, every time step from start (0) to the end of the simulation
- `11:11` only once at time step 11
- `10:100:2` every second time step between steps 10 and 100 (included)
- `42,30:50:10`: at steps 30 40 42 50 84 126 168 ...
- `5,10`: at steps 0 5 10 15 20 25 ... (only executed once per step in overlapping intervals)

2.4.25 Python Postprocessing

In order to further work with the data produced by a plugin during a simulation run, PIConGPU provides python tools that can be used for reading data and visualization. They can be found under `lib/python/picongpu/plugins`.

It is our goal to provide at least three modules for each plugin to make postprocessing as convenient as possible: 1. a data reader (inside the `data` subdirectory) 2. a matplotlib visualizer (inside the `plot_mpl` subdirectory) 3. a jupyter widget visualizer (inside the `jupyter_widgets` subdirectory) for usage in jupyter-notebooks

Further information on how to use these tools can be found at each plugin page.

If you would like to help in developing those classes for a plugin of your choice, please read *python postprocessing*.

References

2.5 TBG

Section author: Axel Huebl

Module author: René Widera

Our tool *template batch generator* (`tbg`) abstracts program runtime options from technical details of supercomputers. On a desktop PC, one can just execute a command interactively and instantaneously. Contrarily on a supercomputer, resources need to be shared between different users efficiently via *job scheduling*. Scheduling on today's supercomputers is usually done via *batch systems* that define various queues of resources.

An unfortunate aspect about batch systems from a user's perspective is, that their usage varies a lot. And naturally, different systems have different resources in queues that need to be described.

PIConGPU runtime options are described in *configuration files* (`.cfg`). We abstract the description of queues, resource acquisition and job submission via *template files* (`.tpl`). For example, a `.cfg` file defines how many *devices* shall be used for computation, but a `.tpl` file calculates how many *physical nodes* will be requested. Also, `.tpl` files takes care of how to spawn a process when scheduled, e.g. with `mpiexec` and which flags for networking details need to be passed. After combining the *machine independent* (portable) `.cfg` file from user input with the *machine dependent* `.tpl` file, `tbg` can submit the requested job to the batch system.

Last but not least, one usually wants to store the input of a simulation with its output. `tbg` conveniently automates this task before submission. The `.tpl` and the `.cfg` files that were used to start the simulation can be found in `<tbg destination dir>/tbg/` and can be used together with the `.param` files from `<tbg destination dir>/input/.../param/` to recreate the simulation setup.

In summary, PIConGPU runtime options in `.cfg` files are portable to any machine. When accessing a machine for the first time, one needs to write template `.tpl` files, abstractly describing how to run PIConGPU on the specific queue(s) of the batch system. We ship such template files already for a set of supercomputers, interactive execution and many common batch systems. See `$PICSRC/etc/picongpu/` and *our list of systems with .profile files* for details.

2.5.1 Usage

```
TBG (template batch generator)
create a new folder for a batch job and copy in all important files

usage: tbg -c [cfgFile] [-s [submitsystem]] [-t [templateFile]]
           [-o "VARNAME1=10 VARNAME2=5"] [-f] [-h]
           [projectPath] destinationPath

-c | --cfg      [file]         - Configuration file to set up batch file.
                                 Default: [cfgFile] via export TBG_CFGFILE
-s | --submit   [command]      - Submit command (qsub, "qsub -h", sbatch, ...)
                                 Default: [submitsystem] via export TBG_SUBMIT
-t | --tpl      [file]         - Template to create a batch file from.
                                 tbg will use stdin, if no file is specified.
                                 Default: [templateFile] via export TBG_TPLFILE
-o                             - Overwrite any template variable:
                                 spaces within the right side of assign are not␣
↪allowed
                                 e.g. -o "VARNAME1=10 VARNAME2=5"
                                 Overwriting is done after cfg file was executed
-f | --force                   - Override if 'destinationPath' exists.
-h | --help                    - Shows help (this output).

[projectPath]                  - Project directory containing source code and
                                 binaries
```

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```
                                  Default: current directory
destinationPath                 - Directory for simulation output.


TBG exports the following variables, which can be used in cfg and tpl files at
any time:
 TBG_jobName                    - name of the job
 TBG_jobNameShort               - short name of the job, without blanks
 TBG_cfgPath                    - absolute path to cfg file
 TBG_cfgFile                    - full absolute path and name of cfg file
 TBG_projectPath                - absolute project path (see optional parameter
                                  projectPath)
 TBG_dstPath                    - absolute path to destination directory
```

2.5.2 .cfg File Macros

Feel free to copy & paste sections of the files below into your `.cfg`, e.g. to configure complex plugins:

```
# Copyright 2014-2021 Felix Schmitt, Axel Huebl, Richard Pausch, Heiko Burau,
#                     Franz Poeschel, Sergei Bastrakov
#
# This file is part of PIConGPU.
#
# PIConGPU is free software: you can redistribute it and/or modify
# it under the terms of the GNU General Public License as published by
# the Free Software Foundation, either version 3 of the License, or
# (at your option) any later version.
#
# PIConGPU is distributed in the hope that it will be useful,
# but WITHOUT ANY WARRANTY; without even the implied warranty of
# MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.  See the
# GNU General Public License for more details.
#
# You should have received a copy of the GNU General Public License
# along with PIConGPU.
# If not, see <http://www.gnu.org/licenses/>.

################################################################################
## This file describes sections and variables for PIConGPU's
## TBG batch file generator.
## These variables basically wrap PIConGPU command line flags.
## To see all flags available for your PIConGPU binary, run
## picongpu --help. The avalable flags depend on your configuration flags.
## Note that this is not meant to be a complete and functioning .cfg file.
##
## Flags that target a specific species e.g. electrons (--e_png) or ions
## (--i_png) must only be used if the respective species is activated (configure␣
↪flags).
##
## If not stated otherwise, variables/flags must not be used more than once!
################################################################################

################################################################################
## Section: Required Variables
## Variables in this secton are necessary for PIConGPU to work properly and should␣
↪not
## be removed. However, you are free to adjust them to your needs, e.g. setting
## the number of GPUs in each dimension.
################################################################################
```

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```
# Batch system walltime
TBG_wallTime="1:00:00"

# Number of devices in each dimension (x,y,z) to use for the simulation
TBG_devices_x=1
TBG_devices_y=2
TBG_devices_z=1

# Size of the simulation grid in cells as "X Y Z"
# note: the number of cells needs to be an exact multiple of a supercell
#       and has to be at least 3 supercells per device,
#       the size of a supercell (in cells) is defined in `memory.param`
TBG_gridSize="128 256 128"

# Number of simulation steps/iterations as "N"
TBG_steps="100"

# disable grid size auto adjustment
TBG_disableGridAutoAdjustment="--autoAdjustGrid off"

################################################################################
## Section: Optional Variables
## You are free to add and remove variables here as you like.
## The only exception is TBG_plugins which is used to forward your variables
## to the TBG program. This variable can be modified but should not be removed!
##
## Please add all variables you define in this section to TBG_plugins.
################################################################################

# Variables which are created by TBG (should be self-descriptive)
TBG_jobName
TBG_jobNameShort
TBG_cfgPath
TBG_cfgFile
TBG_projectPath
TBG_dstPath


# version information on startup
TBG_version="--versionOnce"


# Regex to describe the static distribution of the cells for each device
# default: equal distribution over all devices
# example for -d 2 4 1 -g 128 192 12
TBG_gridDist="--gridDist '64{2}' '64,32{2},64'"


# Specifies whether the grid is periodic (1) or not (0) in each dimension (X,Y,Z).
# Default: no periodic dimensions
TBG_periodic="--periodic 1 0 1"


# Specifies boundaries for given species with a particle pusher, 'e' in the␣
↪example.
# The axis order matches --periodic.
# Default: what is set by --periodic, all offsets 0.
# Supported particle boundary kinds: periodic, absorbing, reflecting, thermal.
# Periodic boundaries require 0 offset, thermal require a positive offset, other␣
↪boundary kinds can have non-negative offsets.
```

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```
# Boundary temperature is set in keV, only affects thermal boundaries.
TBG_particleBoundaries="--e_boundary periodic absorbing thermal --e_boundaryOffset␣
↪0 10 5 --e_boundaryTemperature 0 0 20.0"


# Set absorber type of absorbing boundaries.
# Supported values: exponential, pml (default).
# When changing absorber type, one should normally adjust NUM_CELLS in␣
↪fieldAbsorber.param
TBG_absorber="--fieldAbsorber pml"

# Enables moving window (sliding) in your simulation
TBG_movingWindow="-m"


# Defines when to start sliding the window.
# The window starts sliding at the time required to pass the distance of
# windowMovePoint * (global window size in y) when moving with the speed of light
# Note: beware, there is one "hidden" row of gpus at the y-front, so e.g. when the␣
↪window is enabled
# and this variable is set to 0.75, only 75% of simulation area is used for real␣
↪simulation
TBG_windowMovePoint="--windowMovePoint 0.9"


# stop the moving window after given simulation step
TBG_stopWindow="--stopWindow 1337"


# Set current smoothing.
# Supported values: none (default), binomial
TBG_currentInterpolation="--currentInterpolation binomial"


# Duplicate E and B field storage inside field background to improve performance␣
↪at cost of additional memory
TBG_fieldBackground="--fieldBackground.duplicateFields"


# Allow two MPI ranks to use one compute device.
TBG_ranksPerDevice="--numRanksPerDevice 2"

################################################################################
## Placeholder for multi data plugins:
##
## placeholders must be substituted with the real data name
##
## <species> = species name e.g. e (electrons), i (ions)
## <field>  = field names e.g. FieldE, FieldB, FieldJ
################################################################################

# The following flags are available for the radiation plugin.
# For a full description, see the plugins section in the online wiki.
#--<species>_radiation.period     Radiation is calculated every .period steps.␣
↪Currently 0 or 1
#--<species>_radiation.dump     Period, after which the calculated radiation data␣
↪should be dumped to the file system
#--<species>_radiation.lastRadiation     If flag is set, the spectra summed␣
↪between the last and the current dump-time-step are stored
#--<species>_radiation.folderLastRad     Folder in which the summed spectra are␣
↪stored
```

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```
#--<species>_radiation.totalRadiation     If flag is set, store spectra summed␣
↪from simulation start till current time step
#--<species>_radiation.folderTotalRad     Folder in which total radiation spectra␣
↪are stored
#--<species>_radiation.start     Time step to start calculating the radition
#--<species>_radiation.end     Time step to stop calculating the radiation
#--<species>_radiation.radPerGPU     If flag is set, each GPU stores its own␣
↪spectra without summing the entire simulation area
#--<species>_radiation.folderRadPerGPU     Folder where the GPU specific spectras␣
↪are stored
#--<species>_radiation.numJobs     Number of independent jobs used for the␣
↪radiation calculation.
TBG_radiation="--<species>_radiation.period 1 --<species>_radiation.dump 2 --
↪<species>_radiation.totalRadiation \
               --<species>_radiation.lastRadiation --<species>_radiation.start␣
↪2800 --<species>_radiation.end 3000"

# The following flags are available for the transition radiation plugin.
# For a full description, see the plugins section in the online documentation.
#--<species>_transRad.period   Gives the number of time steps between which the␣
↪radiation should be calculated.
TBG_transRad="--<species>_transRad.period 1000"

# The following flags are available for the xrayScattering plugin.
# For a full description, see the plugins section in the online documentation.
#--<species>_xrayScattering.period    Period at which the plugin is enabled.
#--<species>_xrayScattering.outputPeriod    Period at which the accumulated␣
↪amplitude is written to the output file.
#--<species>_xrayScattering.qx_max    Upper bound of reciprocal space range in qx␣
↪direction.
#--<species>_xrayScattering.qy_max    Upper bound of reciprocal space range in qy␣
↪direction.
#--<species>_xrayScattering.qx_max    Lower bound of reciprocal space range in qx␣
↪direction.
#--<species>_xrayScattering.qy_max    Lower bound of reciprocal space range in qy␣
↪direction.
#--<species>_xrayScattering.n_qx    Number of scattering vectors needed to be␣
↪calculated in qx direction.
#--<species>_xrayScattering.n_qy    Number of scattering vectors needed to be␣
↪calculated in qy direction.
#--<species>_xrayScattering.file    Output file name. Default is `<species>_
↪xrayScatteringOutput`.
#--<species>_xrayScattering.ext    `openPMD` filename extension. This controls the␣
↪backend picked by the `openPMD` API. Default is `bp` for adios2 backend.
#--<species>_xrayScattering.memoryLayout    Possible values: `mirror` and `split`.␣
↪Output can be mirrored on all Host+Device pairs or uniformly split, in chunks,␣
↪over all nodes.
TBG_<species>_xrayScattering="--<species>_xrayScattering.period 1 --e_
↪xrayScattering.outputPeriod 10 \
                  --e_xrayScattering.n_qx 512 --e_xrayScattering.n_qy 512 \
                  --e_xrayScattering.qx_min 0 --e_xrayScattering.qx_max 1 \
                  --e_xrayScattering.qy_min -1 --e_xrayScattering.qy_max 1 \
                  --e_xrayScattering.memoryLayout split"

# Create 2D images in PNG format every .period steps.
# The slice plane is defined using .axis [yx,yz] and .slicePoint (offset from␣
↪origin
# as a float within [0.0,1.0].
# The output folder can be set with .folder.
# Can be used more than once to print different images, e.g. for YZ and YX planes.
TBG_<species>_pngYZ="--<species>_png.period 10 --<species>_png.axis yz --<species>_
↪png.slicePoint 0.5 --<species>_png.folder pngElectronsYZ"
```

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```
TBG_<species>_pngYX="--<species>_png.period 10 --<species>_png.axis yx --<species>_
↪png.slicePoint 0.5 --<species>_png.folder pngElectronsYX"

# Enable macro particle merging
TBG_<species>_merger="--<species>_merger.period 100 --<species>_merger.
↪minParticlesToMerge 8 --<species>_merger.posSpreadThreshold 0.2 --<species>_
↪merger.absMomSpreadThreshold 0.01"

# Enable probabilistic version of particle merging
TBG_<species>_randomizedMerger="--<species>_randomizedMerger.period 100 --<species>
↪_randomizedMerger.maxParticlesToMerge 8                    \
                               --<species>_randomizedMerger.ratioDeletedParticles␣
↪0.9 --<species>_randomizedMerger.posSpreadThreshold 0.01 \
                               --<species>_randomizedMerger.momSpreadThreshold  0.
↪0005"

# Notification period of position plugin (single-particle debugging)
TBG_<species>_pos_dbg="--<species>_position.period 1"


# Create a particle-energy histogram [in keV] per species for every .period steps
TBG_<species>_histogram="--<species>_energyHistogram.period 500 --<species>_
↪energyHistogram.binCount 1024     \
                         --<species>_energyHistogram.minEnergy 0 --<species>_
↪energyHistogram.maxEnergy 500000 \
                         --<species>_energyHistogram.filter all"


# Calculate a 2D phase space
# - momentum range in m_<species> c
TBG_<species>_PSxpx="--<species>_phaseSpace.period 10 --<species>_phaseSpace.
↪filter all --<species>_phaseSpace.space x --<species>_phaseSpace.momentum px --
↪<species>_phaseSpace.min -1.0 --<species>_phaseSpace.max 1.0"
TBG_<species>_PSxpz="--<species>_phaseSpace.period 10 --<species>_phaseSpace.
↪filter all --<species>_phaseSpace.space x --<species>_phaseSpace.momentum pz --
↪<species>_phaseSpace.min -1.0 --<species>_phaseSpace.max 1.0"
TBG_<species>_PSypx="--<species>_phaseSpace.period 10 --<species>_phaseSpace.
↪filter all --<species>_phaseSpace.space y --<species>_phaseSpace.momentum px --
↪<species>_phaseSpace.min -1.0 --<species>_phaseSpace.max 1.0"
TBG_<species>_PSypy="--<species>_phaseSpace.period 10 --<species>_phaseSpace.
↪filter all --<species>_phaseSpace.space y --<species>_phaseSpace.momentum py --
↪<species>_phaseSpace.min -1.0 --<species>_phaseSpace.max 1.0"
TBG_<species>_PSypz="--<species>_phaseSpace.period 10 --<species>_phaseSpace.
↪filter all --<species>_phaseSpace.space y --<species>_phaseSpace.momentum pz --
↪<species>_phaseSpace.min -1.0 --<species>_phaseSpace.max 1.0"

# Write out slices of field data for every .period step
TBG_EField_slice="--E_slice.period 100 --E_slice.fileName sliceE --E_slice.plane 2␣
↪--E_slice.slicePoint 0.5"
TBG_BField_slice="--B_slice.period 100 --B_slice.fileName sliceB --B_slice.plane 2␣
↪--B_slice.slicePoint 0.5"
TBG_JField_slice="--J_slice.period 100 --J_slice.fileName sliceJ --J_slice.plane 2␣
↪--J_slice.slicePoint 0.5"

# Sum up total energy every .period steps for
# - species   (--<species>_energy)
# - fields    (--fields_energy)
TBG_sumEnergy="--fields_energy.period 10 --<species>_energy.period 10 --<species>_
↪energy.filter all"
```

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```
# Count the number of macro particles per species for every .period steps
TBG_macroCount="--<species>_macroParticlesCount.period 100"


# Count makro particles of a species per super cell
TBG_countPerSuper="--<species>_macroParticlesPerSuperCell.period 100 --<species>_
↪macroParticlesPerSuperCell.period 100"


# Dump simulation data (fields and particles) via the openPMD API.
# Data is dumped every .period steps to the fileset .file.
TBG_openPMD="--openPMD.period 100   \
             --openPMD.file simOutput \
             --openPMD.ext bp \
             --openPMD.json '{ \"adios2\": { \"engine\": { \"type\": \"file\", \
↪"parameters\": { \"BufferGrowthFactor\": \"1.2\", \"InitialBufferSize\": \"2GB\"␣
↪} } } }'"
# Further control over the backends used in the openPMD plugins is available
# through the mechanisms exposed by the openPMD API:
# * environment variables
# * JSON-formatted configuration string
# Further information on both is retrieved from the official documentation
# https://openpmd-api.readthedocs.io

# Create a checkpoint that is restartable every --checkpoint.period steps
#   http://git.io/PToFYg
TBG_checkpoint="--checkpoint.period 1000"
# Select the backend for the checkpoint, available are openPMD
#    --checkpoint.backend openPMD
# Available backend options are exactly as in --openPMD.* and can be set
# via:
#   --checkpoint.<IO-backend>.* <value>
# e.g.:
#   --checkpoint.openPMD.dataPreparationStrategy doubleBuffer

# Restart the simulation from checkpoint created using TBG_checkpoint
TBG_restart="--checkpoint.restart"
# Try to restart if a checkpoint is available else start the simulation from␣
↪scratch.
TBG_tryrestart="--checkpoint.tryRestart"
# Select the backend for the restart (must fit the created checkpoint)
#    --checkpoint.restart.backend openPMD
# By default, the last checkpoint is restarted if not specified via
#   --checkpoint.restart.step 1000
# To restart in a new run directory point to the old run where to start from
#   --checkpoint.restart.directory /path/to/simOutput/checkpoints

# Presentation mode: loop a simulation via restarts
#   does either start from 0 again or from the checkpoint specified with
#   --checkpoint.restart.step as soon as the simulation reached the last time step;
#   in the example below, the simulation is run 5000 times before it shuts down
# Note: does currently not work with `Radiation` plugin
TBG_restartLoop="--checkpoint.restart.loop 5000"

# Live in situ visualization using ISAAC
#   Initial period in which a image shall be rendered
#     --isaac.period PERIOD
#   Name of the simulation run as seen for the connected clients
#     --isaac.name NAME
#   URL of the server
#     --isaac.url URL
```

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```
#   Number from 1 to 100 decribing the quality of the transceived jpeg image.
#   Smaller values are faster sent, but of lower quality
#     --isaac.quality QUALITY
#   Resolution of the rendered image. Default is 1024x768
#     --isaac.width WIDTH
#     --isaac.height HEIGHT
#   Pausing directly after the start of the simulation
#     --isaac.directPause
#   By default the ISAAC Plugin tries to reconnect if the sever is not available
#   at start or the servers crashes. This can be deactivated with this option
#     --isaac.reconnect false
#   Enable and write benchmark results into the given file.
#     --isaac.timingsFilename benchResults.txt
TBG_isaac="--isaac.period 1 --isaac.name !TBG_jobName --isaac.url <server_url>"
TBG_isaac_quality="--isaac.quality 90"
TBG_isaac_resolution="--isaac.width 1024 --isaac.height 768"
TBG_isaac_pause="--isaac.directPause"
TBG_isaac_reconnect="--isaac.reconnect false"

# Print the maximum charge deviation between particles and div E to textfile
↪'chargeConservation.dat':
TBG_chargeConservation="--chargeConservation.period 100"

# Particle calorimeter: (virtually) propagates and collects particles to infinite␣
↪distance
TBG_<species>_calorimeter="--<species>_calorimeter.period 100 --<species>_
↪calorimeter.openingYaw 90 --<species>_calorimeter.openingPitch 30
                           --<species>_calorimeter.numBinsEnergy 32 --<species>_
↪calorimeter.minEnergy 10 --<species>_calorimeter.maxEnergy 1000
                           --<species>_calorimeter.logScale 1 --<species>_calorimeter.
↪file filePrefix --<species>_calorimeter.filter all"

# Resource log: log resource information to streams or files
# set the resources to log by --resourceLog.properties [rank, position,␣
↪currentStep, particleCount, cellCount]
# set the output stream by --resourceLog.stream [stdout, stderr, file]
# set the prefix of filestream --resourceLog.prefix [prefix]
# set the output format by (pp == pretty print) --resourceLog.format jsonpp [json,
↪jsonpp,xml,xmlpp]
# The example below logs all resources for each time step to stdout in the pretty␣
↪print json format
TBG_resourceLog="--resourceLog.period 1 --resourceLog.stream stdout
                 --resourceLog.properties rank position currentStep particleCount␣
↪cellCount
                 --resourceLog.format jsonpp"

################################################################################
## Section: Program Parameters
## This section contains TBG internal variables, often composed from required
## variables. These should not be modified except when you know what you are doing!
################################################################################

# Number of compute devices in each dimension as "X Y Z"
TBG_deviceDist="!TBG_devices_x !TBG_devices_y !TBG_devices_z"


# Combines all declared variables. These are passed to PIConGPU as command line␣
↪flags.
# The program output (stdout) is stored in a file called output.stdout.
TBG_programParams="-d !TBG_deviceDist \
                   -g !TBG_gridSize   \
```

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```
                  -s !TBG_steps      \
                  !TBG_plugins"

# Total number of devices
TBG_tasks="$(( TBG_devices_x * TBG_devices_y * TBG_devices_z ))"
```

2.5.3 Batch System Examples

Section author: Axel Huebl, Richard Pausch

Slurm

Slurm is a modern batch system, e.g. installed on the Taurus cluster at TU Dresden, Hemera at HZDR, Cori at NERSC, among others.

Job Submission

PIConGPU job submission on the *Taurus* cluster at *TU Dresden*:

- `tbg -s sbatch -c etc/picongpu/0008gpus.cfg -t etc/picongpu/taurus-tud/k80.tpl $SCRATCH/runs/test-001`

Job Control

- interactive job:
  - `salloc --time=1:00:00 --nodes=1 --ntasks-per-node=2 --cpus-per-task=8 --partition gpu-interactive`
  - e.g. `srun "hostname"`
  - GPU allocation on taurus requires an additional flag, e.g. for two GPUs `--gres=gpu:2`
- details for my jobs:
  - `scontrol -d show job 12345` all details for job with <job id> `12345`
  - `squeue -u $(whoami) -l` all jobs under my user name
- details for queues:
  - `squeue -p queueName -l` list full queue
  - `squeue -p queueName --start` (show start times for pending jobs)
  - `squeue -p queueName -l -t R` (only show running jobs in queue)
  - `sinfo -p queueName` (show online/offline nodes in queue)
  - `sview` (alternative on taurus: `module load llview` and `llview`)
  - `scontrol show partition queueName`
- communicate with job:
  - `scancel <job id>` abort job
  - `scancel -s <signal number> <job id>` send signal or signal name to job
  - `scontrol update timelimit=4:00:00 jobid=12345` change the walltime of a job
  - `scontrol update jobid=12345 dependency=afterany:54321` only start job `12345` after job with id `54321` has finished

  - `scontrol hold <job id>` prevent the job from starting
  - `scontrol release <job id>` release the job to be eligible for run (after it was set on hold)

LSF

LSF (for *Load Sharing Facility*) is an IBM batch system (`bsub`/BSUB). It is used, e.g. on Summit at ORNL.

Job Submission

PIConGPU job submission on the *Summit* cluster at *Oak Ridge National Lab*:

- `tbg -s bsub -c etc/picongpu/0008gpus.cfg -t etc/picongpu/summit-ornl/gpu.tpl $PROJWORK/$proj/test-001`

Job Control

- interactive job:
  - `bsub -P $proj -W 2:00 -nnodes 1 -Is /bin/bash`
- details for my jobs:
  - `bjobs 12345` all details for job with <job id> `12345`
  - `bjobs [-l]` all jobs under my user name
  - `jobstat -u $(whoami)` job eligibility
  - `bjdepinfo 12345` job dependencies on other jobs
- details for queues:
  - `bqueues` list queues
- communicate with job:
  - `bkill <job id>` abort job
  - `bpeek [-f] <job id>` peek into `stdout`/`stderr` of a job
  - `bkill -s <signal number> <job id>` send signal or signal name to job
  - `bchkpnt` and `brestart` checkpoint and restart job (untested/unimplemented)
  - `bmod -W 1:30 12345` change the walltime of a job (currently not allowed)
  - `bstop <job id>` prevent the job from starting
  - `bresume <job id>` release the job to be eligible for run (after it was set on hold)

References

- https://www.olcf.ornl.gov/for-users/system-user-guides/summit/summit-user-guide/#running-jobs
- https://www.ibm.com/support/knowledgecenter/en/SSETD4/product_welcome_platform_lsf.html

2.6 Python

This section contains python utilities for more comfortable working with PIConGPU.

2.6.1 Memory Calculator

To aid you in the planning and setup of your simulation PIConGPU provides python tools for educated guesses on simulation parameters. They can be found under `lib/python/picongpu/utils`.

Calculate the memory requirement per device.

```
from picongpu.utils import MemoryCalculator
```

class picongpu.utils.memory_calculator.**MemoryCalculator**(*n_x*, *n_y*, *n_z*, *precision_bits=32*)

Memory requirement calculation tool for PIConGPU

Contains calculation for fields, particles, random number generator and the calorimeter plugin. In-situ methods other than the calorimeter so far use up negligible amounts of memory on the device.

__init__(*n_x*, *n_y*, *n_z*, *precision_bits=32*)

Class constructor

Parameters

- **n_x** (*int*) – number of cells in x direction (per device)
- **n_y** (*int*) – number of cells in y direction (per device)
- **n_z** (*int*) – number of cells in z direction (per device)
- **precision_bits** (*int*) – floating point precision for PIConGPU run

mem_req_by_calorimeter(*n_energy*, *n_yaw*, *n_pitch*, *value_size=None*)

Memory required by the particle calorimeter plugin. Each of the (`n_energy` x `n_yaw` x `n_pitch`) bins requires a value (32/64 bits). The whole calorimeter is represented twice on each device, once for particles in the simulation and once for the particles that leave the box.

Parameters

- **n_energy** (*int*) – number of bins on the energy axis
- **n_yaw** (*int*) – number of bins for the yaw angle
- **n_pitch** (*int*) – number of bins for the pitch angle
- **value_size** (*int*) – value size in particle calorimeter {unit: byte} (default: 4)

Returns **req_mem** – required memory {unit: bytes} per device

Return type int

mem_req_by_fields(*n_x=None*, *n_y=None*, *n_z=None*, *field_tmp_slots=1*, *particle_shape_order=2*, *sim_dim=3*, *pml_n_x=0*, *pml_n_y=0*, *pml_n_z=0*)

Memory reserved for fields on each device

Parameters

- **n_x** (*int*) – number of cells in x direction (per device)
- **n_y** (*int*) – number of cells in y direction (per device)
- **n_z** (*int*) – number of cells in z direction (per device)
- **field_tmp_slots** (*int*) – number of slots for temporary fields (see PIConGPU `memory.param` : `fieldTmpNumSlots`)
- **particle_shape_order** (*int*) – numerical order of the assignment function of the chosen particle shape CIC : order 1 TSC : order 2 PQS : order 3 PCS : order 4 (see PIConGPU `species.param`)
- **sim_dim** (*int*) – simulation dimension (available for PIConGPU: 2 and 3)
- **pml_n_x** (*int*) – number of PML cells in x direction, combined for both sides
- **pml_n_y** (*int*) – number of PML cells in y direction, combined for both sides

- **pml_n_z** (*int*) – number of PML cells in z direction, combined for both sides

Returns **req_mem** – required memory {unit: bytes} per device

Return type int

mem_req_by_particles(*target_n_x=None*, *target_n_y=None*, *target_n_z=None*, *num_additional_attributes=0*, *particles_per_cell=2*, *sim_dim=3*)

Memory reserved for all particles of a species on a device. We currently neglect the constant species memory.

Parameters

- **target_n_x** (*int*) – number of cells in x direction containing the target
- **target_n_y** (*int*) – number of cells in y direction containing the target
- **target_n_z** (*int*) – number of cells in z direction containing the target
- **num_additional_attributes** (*int*) – number of additional attributes like e.g. `boundElectrons`
- **particles_per_cell** (*int*) – number of particles of the species per cell
- **sim_dim** (*int*) – simulation dimension (available for PIConGPU: 2 and 3)

Returns **req_mem** – required memory {unit: bytes} per device and species

Return type int

mem_req_by_rng(*n_x=None*, *n_y=None*, *n_z=None*, *generator_method='XorMin'*)

Memory reserved for the random number generator state on each device.

Check `random.param` for a choice of random number generators. If you find that your required RNG state is large (> 300 MB) please see `memory.param` for a possible adjustment of the `reservedGpuMemorySize`.

Parameters

- **n_x** (*int*) – number of cells in x direction (per device)
- **n_y** (*int*) – number of cells in y direction (per device)
- **n_z** (*int*) – number of cells in z direction (per device)
- **generator_method** (*str*) – random number generator method - influences the state size per cell possible options: "XorMin", "MRG32k3aMin", "AlpakaRand" - (GPU default: "XorMin") - (CPU default: "AlpakaRand")

Returns **req_mem** – required memory {unit: bytes} per device

Return type int

2.7 Example Setups

2.7.1 Bremsstrahlung: Emission of Bremsstrahlung from Laser-Foil Interaction

Section author: Heiko Burau <h.burau (at) hzdr.de>

Module author: Heiko Burau <h.burau (at) hzdr.de>

This is a simulation of a flat solid density target hit head-on by a high-intensity laser pulse. At the front surface free electrons are accelerated up to ultra relativistic energies and start travelling through the bulk then. Meanwhile, due to ion interaction, the hot electrons lose a small fraction of their kinetic energy in favor of emission of Bremsstrahlung-photons. Passing over the back surface hot electrons are eventually reflected and re-enter the foil in opposite direction. Because of the ultra-relativistic energy Bremsstrahlung (BS) is continuously emitted mainly along the direction of motion of the electron. The BS-module models the electron-ion scattering as three

single processes, including electron deflection, electron deceleration and photon creation with respect to the emission angle. Details of the implementation and the numerical model can be found in [BurauDipl]. Details of the theoretical description can be found in [Jackson] and [Salvat].

This 2D test simulates a laser pulse of a_0=40, lambda=0.8µm, w0=1.5µm in head-on collision with a fully pre-ionized gold foil of 2µm thickness.

Checks

- check appearence of photons moving along (forward) and against (backward) the incident laser pulse direction.
- check photon energy spectrum in both directions for the forward moving photons having a higher energy.

References

2.7.2 Bunch: Thomson scattering from laser electron-bunch interaction

Section author: Richard Pausch <r.pausch (at) hzdr.de>

Module author: Richard Pausch <r.pausch (at) hzdr.de>, Rene Widera <r.widera (at) hzdr.de>

This is a simulation of an electron bunch that collides head-on with a laser pulse. Depending on the number of electrons in the bunch, their momentum and their distribution and depending on the laser wavelength and intensity, the emitted radiation differs. A general description of this simulation can be found in [PauschDipl]. A detailed analysis of this bunch simulation can be found in [Pausch13]. A theoretical study of the emitted radiation in head-on laser electron collisions can be found in [Esarey93].

This test simulates an electron bunch with a relativistic gamma factor of gamma=5.0 and with a laser with a_0=1.0. The resulting radiation should scale with the number of real electrons (incoherent radiation).

References

2.7.3 Empty: Default PIC Algorithm

Section author: Axel Huebl <a.huebl (at) hzdr.de>

This is an "empty" example, initializing a default particle-in-cell cycle with default algorithms [BirdsallLangdon] [HockneyEastwood] but without a specific test case. When run, it iterates a particle-in-cell algorithm on a vacuum without particles or electro-magnetic fields initialized, which are the default `.param` files in `include/picongpu/param/`.

This is a case to demonstrate and test these defaults are still (syntactically) working. In order to set up your own simulation, there is no need to overwrite all `.param` files but only the ones that are different from the defaults. As an example, just overwrite the default laser (none) and initialize a species with a density distribution.

References

2.7.4 FoilLCT: Ion Acceleration from a Liquid-Crystal Target

Section author: Axel Huebl

Module author: Axel Huebl, T. Kluge

The following example models a laser-ion accelerator in the [TNSA] regime. An optically over-dense target ($n_{\mathrm{max}} = 192 n_{\mathrm{c}}$) consisting of a liquid-crystal material *8CB* (4-octyl-4'-cyanobiphenyl) $C_{21}H_{25}N$ is used [LCT].

Irradiated with a high-power laser pulse with $a_0 = 5$ the target is assumed to be partly pre-ionized due to realistic laser contrast and pre-pulses to C^{2+}, H^{+} and N^{2+} while being slightly expanded on its surfaces (modeled as

exponential density slope). The overall target is assumed to be initially quasi-neutral and the *8CB* ion components are are not demixed in the surface regions. Surface contamination with, e.g. water vapor is neglected.

The laser is assumed to be in focus and approximated as a plane wave with temporally Gaussian intensity envelope of $\tau_I^{\mathrm{FWHM}} = 25$ fs.

This example is used to demonstrate:

- an ion acceleration setup with
- *composite, multi ion-species target material*
- *quasi-neutral initial conditions*
- ionization models for *field ionization* and *collisional ionization*

with PIConGPU.

References

2.7.5 KelvinHelmholtz: Kelvin-Helmholtz Instability

Section author: Axel Huebl <a.huebl (at) hzdr.de>

Module author: Axel Huebl <a.huebl (at) hzdr.de>, E. Paulo Alves, Thomas Grismayer

This example simulates a shear-flow instability known as the Kelvin-Helmholtz Instability in a near-relativistic setup as studied in [Alves12], [Grismayer13], [Bussmann13]. The default setup uses a pre-ionized quasi-neutral hydrogen plasma. Modifiying the ion species' mass to resample positrons instead is a test we perform regularly to control numerical heating and charge conservation.

References

2.7.6 LaserWakefield: Laser Electron Acceleration

Section author: Axel Huebl <a.huebl (at) hzdr.de>

Module author: Axel Huebl <a.huebl (at) hzdr.de>, René Widera, Heiko Burau, Richard Pausch, Marco Garten

Setup for a laser-driven electron accelerator [TajimaDawson] in the blowout regime of an underdense plasma [Modena] [PukhovMeyerterVehn]. A short (fs) laser beam with ultra-high intensity (a_0 >> 1), modeled as a finite Gaussian beam is focussed in a hydrogen gas target. The target is assumed to be pre-ionized with negligible temperature. The relevant area of interaction is followed by a co-moving window, in whose time span the movement of ions is considered irrelevant which allows us to exclude those from our setup.

This is a demonstration setup to get a visible result quickly and test available methods and I/O. The plasma gradients are unphysically high, the resolution of the laser wavelength is seriously bad, the laser parameters (e.g. pulse length, focusing) are challening to achieve technically and interaction region is too close to the boundaries of the simulation box. Nevertheless, this setup will run on a single GPU in full 3D in a few minutes, so just enjoy running it and interact with our plugins!

References

2.7.7 TransitionRadiation : Transtion Radiation

Section author: Finn-Ole Carstens <f.carstens (at) hzdr.de>

This example simulates the coherent and incoherent transition radiation created by an electron bunch in-situ. The implemented transition radiation follows the studies from [Schroeder2004] and [Downer2018]. The transition radiation is computed for an infinitely large interface perpendicular to the y-axis of the simulation.

The electron bunch in this setup is moving with a 45° angle in the x-y plane with a Lorentz-factor of $gamma = 100$. The bunch has a Gaussian distribution with $sigma_y = 3.0 mu m$. The results can be interpreted with the according python script *lib/python/picongpu/plugins/plot_mpl/transition_radiation_visualizer.py*.

References

2.7.8 WarmCopper: Average Charge State Evolution of Copper Irradiated by a Laser

Section author: Axel Huebl <a.huebl (at) hzdr.de>

Module author: Axel Huebl <a.huebl (at) hzdr.de>, Hyun-Kyung Chung

This setup initializes a homogenous, non-moving, copper block irradiated by a laser with 10^18 W/cm^3 as a benchmark for [SCFLY][1] atomic population dynamics. We follow the setup from [FLYCHK] page 10, figure 4 assuming a quasi 0D setup with homogenous density of a 1+ ionized copper target. The laser (not modeled) already generated a thermal electron density at 10, 100 or 1000 eV and a delta-distribution like "hot" electron distribution with 200 keV (directed stream). The observable of interest is <Z> over time of the copper ions. For low thermal energies, collisional excitation, de-excitation and recombinations should be sufficient to reach the LTE state after about 0.1-1 ps. For higher initial temperatures, radiative rates get more relevant and the Non-LTE steady-state solution can only be reached correctly when also adding radiative rates.

Note: FLYlite is still in development!

References

2.8 Workflows

This section contains typical user workflows and best practices.

2.8.1 Adding Laser

Section author: Sergei Bastrakov

There are several alternative ways of adding an incoming laser (or any source of electromagnetic field) to a PIConGPU simulation:

1. selecting a laser profile in *laser.param*
2. enabling an incident field source in *incidentField.param*
3. using field or current background in *fieldBackground.param*

These ways operate independently of one another, each has its features and limitations. All but the current background one are fully accurate only for the standard Yee field solver. For other field solver types, a user should evaluate the inaccuracies introduced.

The functioning of the laser (the first way) is covered in more detail in the following class:

template<uint32_t **T_initPlaneY**>
class BaseFunctor

Base device-side functor for laser profile implementations.

Stores common data for all such implementations. Implements the logic of contributing the stored value to the grid value of E. Has two modes of operation depending on T_initPlaneY: a hard and a mixed hard-soft source.

[1] In PIConGPU, we generally refer to the implemented subset of *SCFLY* (solving Non-LTE population kinetics) as *FLYlite*.

For the T_initPlaneY == 0 case, our laser is a classic hard source: E(y=0, t) = E_source(y=0, t). A notable disadvantage of hard sources is that they are not transparent for incoming waves (e.g. reflected from a target) while the laser is being generated as controlled by its pulse length. More details on hard sources are given in section 5.1 of the book A. Taflove, S.C. Hagness. Computational Electrodynamics. The Finite-Difference Time-Domain Method. Third Edition. Artech house, Boston (2005).

Generally, hard-setting E at a hyperplane y=0 generates E waves going in +y and -y directions. Those E waves will propagate to both sides symmetrically, both theoretically and in an FDTD solver. So the corresponding field (only part generated by the source) E(y) is even wrt y: E(y) = E(-y). Therefore the FDTD-solved resulting B field is odd: B(y) = -B(-y), and particularly B(0) = 0. These relations simply follow from the way of setting the source and properties of FDTD.

The above paragraph applies to a theoretical case of FDTD-propagating fields everywhere. However, it is not exactly what happens in a PIConGPU simulation. In PIConGPU, grid values to the left from the y = 0 plane are not updated by a field solver. So there will be no left-propagating wave in a simulation, only the right-propagating one. Note that it is only due to not applying a field solver, not because of a reflecting boundary. For the classic Yee solver, this scheme is completely fine. Updates for all grid values with y > 0 use only "good" values with y >= 0. These include Bx, Bz in the cell starting at y = 0 as they are located as y = dy/2. And Ex, Ez values at exactly y = 0 are overwritten with the hard source. However, this scheme is not fully accurate for wider stencils used in FDTD. In that case, some updates would use "bad" values from the y < 0 area, that are always kept 0. Thus, the laser with initPlaneY = 0 is only fully accurate with the classic Yee solver.

For the T_initPlaneY > 0 case, our laser is a mixed hard-soft source. It also only affects E, but following E(y=0, t) += coefficient * E_source(y=0, t). Beware a principle difference of this scheme from classic soft sources. Those are formulated using currents J, M derived from B_source, E_source. The soft source scheme (in equivalent TF/SF formulation) is implemented in incidentField and is explained there in more detail.

However, the laser in question operates differently. We merely fit the coefficient so that the combination of source application and field solver produces expected values in the y > T_initPlaneY area. Our coefficient value matches that in (33) with alpha = 2 in M. Mansourabadi, A. Pourkazemi. FDTD Hard Source and Soft Source Reviews and Modifications. Progress In Electromagnetics Research C, Vol. 3, 143-160, 2008. doi:10.2528/PIERC08032302. (However they unconventionally call this scheme simply "soft source"). Similarly to the hard source, the scheme implies the laser-induced B values are odd wrt the source. Same as in the previous case, all grid values with y >= 0 will be updated by a field solver. There will be a left-propagating wave in the 0 <= y < T_initPlaneY area generated by the source. This area should normally be excluded when analysing the results. A field absorber should be used at the y_min border to avoid significant influence of this region on the rest of the simulation volume. Note that unlike the hard source case, this source is transparent for incoming waves. Same as the hard-source case, this scheme is fully accurate only for the classic Yee solver.

Template Parameters

- `T_initPlaneY`: laser initialization plane in y, value in cells in the global coordinates

2.8.2 Boundary Conditions

Section author: Sergei Bastrakov, Lennert Sprenger

Two kinds of boundary conditions are supported: periodic and absorbing. They are set in a *.cfg file* with option `--periodic <x> <y> <z>`. Value 0 corresponds to absorbing boundaries along the axis (used by default), 1 corresponds to periodic. The same boundary condition kind is applied for all particles species and fields, on both sides.

Particles

By default, boundary kinds match the value of `--periodic` and so are either periodic or absorbing. For species with a particle pusher, it can be overridden with option *–<prefix>_boundary <x> <y> <z>*. The supported boundary kinds are: periodic, absorbing, reflecting, and thermal.

Currently only the following combinations of field and particle boundaries are supported. When fields are periodic along an axis, boundaries for all species must be periodic along this axis. When fields are absorbing (non-periodic), species must be absorbing, reflecting, or thermal.

By default, the particle boundaries are applied at the global domain boundaries. For absorbing boundaries it means that particles will exist in the field absorbing area. This may be undesired for simulations with Perfectly Matched Layers (see below). A user can change the boundary application area by setting an offset with the option *–<prefix>_boundaryOffset <x> <y> <z>*. The *boundaryOffset* is in terms of whole cells, so integers are expected. It sets an offset inwards from the global domain boundary. Periodic boundaries only allow 0 offset, thermal boundaries require a positive offset, and other kinds support non-negative offsets.

Boundary temperature for thermal boundaries, in keV, is set with option *–<prefix>_boundaryTemperature <x> <y> <z>*.

For example, reflecting and thermal boundary conditions for species *e* are configured by *–e_boundary reflecting thermal reflecting –e_boundaryOffset 0 1 10 –e_boundaryTemperature 0.0 20.0 0.0*

Particles are not allowed to be outside the boundaries for the respective species. (For the periodic case, there are no boundaries in that sense.) After species are initialized, all outer particles will be deleted. During the simulation, the crossing particles will be handled by boundary condition implementations and moved or deleted as a result.

The internal treatment of particles in the guard area is controlled by the `boundaryCondition` flag in *speciesDefinition.param*. However, this option is for expert users and generally should not be modified. To set physical boundary conditions, use the command-line option described above.

Fields

Periodic boundary conditions for fields do not allow customization or variants. The rest of the section concerns absorbing boundaries.

For the absorbing boundaries, there is a virtual field absorber layer inside the global simulation area near its boundaries. Field values in the layer are treated differently from the rest, by a combination of a field solver and a field absorber. It causes field dynamics inside the absorber layer to differ from that in a vacuum. Otherwise, the affected cells are a normal part of a simulation in terms of indexing, particle handling, and output. It is recommended to avoid, as possible, having particles in the field absorber layer. Ideally, only particles leaving the simulation area are present there, on their way to be absorbed. Note that particle absorption happens at the external surface of the field absorber layer, matching the global simulation area border.

The field absorber mechanism and user-controlled parameters depend on the field absorber kind enabled. It is controlled by command-line option `--fieldAbsorber`. For all absorber kinds, the parameters are controlled by *fieldAbsorber.param*.

By default, the Perfectly Matched Layer (PML) absorber is used. For this absorber, thickness of 8 to 12 cells is recommended. Other absorber parameters can generally be used with default values. PML generally provides much better absorber qualities than the exponential damping absorber.

For the exponential absorber, thickness of about 32 cells is recommended.

2.8.3 Setting the Number of Cells

Section author: Axel Huebl

Together with the grid resolution in *grid.param*, the number of cells in our *.cfg files* determine the overall size of a simulation (box). The following rules need to be applied when setting the number of cells:

Each device needs to:

1. contain an integer *multiple* of supercells
2. at least *three* supercells
3. for non periodic boundary conditions, the number of absorbing boundary cells for devices at the simulation boundary (see *grid.param*) must fit into the local volume

The grid size will be automatically adjusted if the conditions above are not fulfilled. This behavior can be disabled by using the command line option `--autoAdjustGrid off`

Supercell sizes in terms of number of cells are set in *memory.param* and are by default `8x8x4` for 3D3V simulations on GPUs. For 2D3V simulations, `16x16` is usually a good supercell size, however the default is simply cropped to `8x8`, so make sure to change it to get more performance.

2.8.4 Changing the Resolution with a Fixed Target

Section author: Axel Huebl

One often wants to refine an already existing resolution in order to model a setup more precisely or to be able to model a higher density.

1. change cell sizes and time step in *grid.param*
2. change number of GPUs in *.cfg file*
3. change number of *number of cells and distribution over GPUs* in *.cfg file*
4. adjust (transveral) positioning of targets in *density.param*
5. *recompile*

2.8.5 Calculating the Memory Requirement per Device

Section author: Marco Garten

The planning of simulations for realistically sized problems requires a careful estimation of memory usage and is often a trade-off between resolution of the plasma, overall box size and the available resources. The file *memory_calculator.py* contains a class for this purpose.

The following paragraph shows the use of the `MemoryCalculator` for the `4.cfg` setup of the *FoilLCT example* example.

It is an estimate for how much memory is used per device if the whole target would be fully ionized but does not move much. Of course, the real memory usage depends on the case and the dynamics inside the simulation. We calculate the memory of just one device per row of GPUs in laser propagation direction. We hereby assume that particles are distributed equally in the transverse direction like it is set up in the FoilLCT example.

We encourage to try out this script with different settings, to see how they influence the distribution of the total memory requirement between devices.

```
from picongpu.utils import MemoryCalculator
from math import ceil


cell_size = 0.8e-6 / 384.  # 2.083e-9 m
y0 = 0.5e-6  # position of foil front surface (m)
y1 = 1.5e-6  # position of foil rear surface (m)
L = 10e-9  # pre-plasma scale length (m)
L_cutoff = 4 * L  # pre-plasma length (m)

sim_dim = 2
# number of cells in the simulation
Nx_all, Ny_all, Nz_all = 256, 1280, 1
# number of GPU rows in each direction
x_rows, y_rows, z_rows = 2, 2, 1
# number of cells per GPU
Nx, Ny, Nz = Nx_all / x_rows, Ny_all / y_rows, Nz_all / z_rows

vacuum_cells = ceil((y0 - L_cutoff) / cell_size)  # in front of the target
# target cells (between surfaces + pre-plasma)
```

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```
target_cells = ceil((y1 - y0 + 2 * L_cutoff) / cell_size)
# number of cells (y direction) on each GPU row
GPU_rows = [0] * y_rows
cells_to_spread = vacuum_cells + target_cells
# spread the cells on the GPUs
for ii, _ in enumerate(GPU_rows):
    if cells_to_spread >= Ny:
        GPU_rows[ii] = Ny
        cells_to_spread -= Ny
    else:
        GPU_rows[ii] = cells_to_spread
        break
# remove vacuum cells from the front rows
extra_cells = vacuum_cells
for ii, _ in enumerate(GPU_rows):
    if extra_cells >= Ny:
        GPU_rows[ii] = 0
        extra_cells -= Ny
    else:
        GPU_rows[ii] -= extra_cells
        break

pmc = MemoryCalculator(Nx, Ny, Nz)

# typical number of particles per cell which is multiplied later for
# each species and its relative number of particles
N_PPC = 6
# conversion factor to megabyte
megabyte = 1.0 / (1024 * 1024)

target_x = Nx  # full transverse dimension of the GPU
target_z = Nz


def sx(n):
    return {1: "st", 2: "nd", 3: "rd"}.get(n if n < 20
                                           else int(str(n)[-1]), "th")


for row, target_y in enumerate(GPU_rows):
    print("{}{} row of GPUs:".format(row + 1, sx(row + 1)))
    print("* Memory requirement per GPU:")
    # field memory per GPU
    field_gpu = pmc.mem_req_by_fields(Nx, Ny, Nz, field_tmp_slots=2,
                                      particle_shape_order=2, sim_dim=sim_dim)
    print(" + fields: {:.2f} MB".format(
        field_gpu * megabyte))

    # electron macroparticles per supercell
    e_PPC = N_PPC * (
            # H,C,N pre-ionization - higher weighting electrons
            3
            # electrons created from C ionization
            + (6 - 2)
            # electrons created from N ionization
            + (7 - 2)
    )
    # particle memory per GPU - only the target area contributes here
    e_gpu = pmc.mem_req_by_particles(
        target_x, target_y, target_z,
        num_additional_attributes=0,
```

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```
        particles_per_cell=e_PPC
    )
    H_gpu = pmc.mem_req_by_particles(
        target_x, target_y, target_z,
        # no bound electrons since H is pre-ionized
        num_additional_attributes=0,
        particles_per_cell=N_PPC
    )
    C_gpu = pmc.mem_req_by_particles(
        target_x, target_y, target_z,
        num_additional_attributes=1,  # number of bound electrons
        particles_per_cell=N_PPC
    )
    N_gpu = pmc.mem_req_by_particles(
        target_x, target_y, target_z,
        num_additional_attributes=1,
        particles_per_cell=N_PPC
    )
    # memory for calorimeters
    cal_gpu = pmc.mem_req_by_calorimeter(
        n_energy=1024, n_yaw=360, n_pitch=1
    ) * 2  # electrons and protons
    # memory for random number generator states
    rng_gpu = pmc.mem_req_by_rng(Nx, Ny, Nz)

    print(" + species:")
    print("  - e: {:.2f} MB".format(e_gpu * megabyte))
    print("  - H: {:.2f} MB".format(H_gpu * megabyte))
    print("  - C: {:.2f} MB".format(C_gpu * megabyte))
    print("  - N: {:.2f} MB".format(N_gpu * megabyte))
    print(" + RNG states: {:.2f} MB".format(
        rng_gpu * megabyte))
    print(
        " + particle calorimeters: {:.2f} MB".format(
            cal_gpu * megabyte))

    mem_sum = field_gpu + e_gpu + H_gpu + C_gpu + N_gpu + rng_gpu + cal_gpu
    print("* Sum of required GPU memory: {:.2f} MB".format(
        mem_sum * megabyte))
```

This will give the following output:

```
1st row of GPUs:
* Memory requirement per GPU:
 + fields: 4.58 MB
 + species:
  - e: 114.16 MB
  - H: 9.51 MB
  - C: 10.74 MB
  - N: 10.74 MB
 + RNG states: 1.88 MB
 + particle calorimeters: 5.62 MB
* Sum of required GPU memory: 157.23 MB
2nd row of GPUs:
* Memory requirement per GPU:
 + fields: 4.58 MB
 + species:
  - e: 27.25 MB
  - H: 2.27 MB
  - C: 2.56 MB
  - N: 2.56 MB
```

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```
 + RNG states: 1.88 MB
 + particle calorimeters: 5.62 MB
* Sum of required GPU memory: 46.72 MB
```

If you have a machine or cluster node with NVIDIA GPUs you can find out the available memory size by typing `nvidia-smi` on a shell.

2.8.6 Setting the Laser Initialization Cut-Off

Section author: Axel Huebl

Laser profiles for simulation are modeled with a temporal envelope. A common model assumes a Gaussian intensity distribution over time which by definition never sets to zero, so it needs to be cut-off to a reasonable range.

In *laser.param* each profile implements the cut-off to start (and end) initializing the laser profile via a parameter `PULSE_INIT` t_{init} (sometimes also called `RAMP_INIT`). t_{init} is given in units of the `PULSE_LENGTH` τ which is implemented *laser-profile dependent* (but usually as σ_I of the standard Gaussian of intensity $I = E^2$).

For a fixed target in distance d to the lower $y = 0$ boundary of the simulation box, the maximum intensity arrives at time:

$$t_{\text{laserPeakOnTarget}} = \frac{t_{\text{init}} \cdot \tau}{2} + \frac{d}{c_0}$$

or in terms of discrete time steps Δt:

$$\text{step}_{\text{laserPeakOnTarget}} = \frac{t_{\text{laserPeakOnTarget}}}{\Delta t}.$$

Note: Moving the spatial plane of initialization of the laser pulse via `initPlaneY` does not change the formula above. The implementation covers this spatial offset during initialization.

2.8.7 Definition of Composite Materials

Section author: Axel Huebl

The easiest way to define a composite material in PIConGPU is starting relative to an idealized full-ionized electron density. As an example, lets use $C_{21}H_{25}N$ (*"8CB"*) with a plasma density of $n_{\text{e,max}} = 192\, n_{\text{c}}$ contributed by the individual ions relatively as:

- Carbon: $21 \cdot 6/N_{\Sigma\text{e-}}$
- Hydrogen: $25 \cdot 1/N_{\Sigma\text{e-}}$
- Nitrogen: $1 \cdot 7/N_{\Sigma\text{e-}}$

and $N_{\Sigma\text{e-}} = 21_{\text{C}} \cdot 6_{\text{C}^{6+}} + 25_{\text{H}} \cdot 1_{\text{H}^{+}} + 1_{\text{N}} \cdot 7_{\text{N}^{7+}} = 158$.

Set the idealized electron density in *density.param* as a reference and each species' relative `densityRatio` from the list above accordingly in *speciesDefinition.param* (see the input files in the *FoilLCT example* for details).

In order to initialize the electro-magnetic fields self-consistently, read *quasi-neutral initialization*.

2.8.8 Quasi-Neutral Initialization

Section author: Axel Huebl

In order to initialize the electro-magnetic fields self-consistently, one needs to fulfill Gauss's law $\vec{\nabla} \cdot \vec{E} = \frac{\rho}{\epsilon_0}$ (and $\vec{\nabla} \cdot \vec{B} = 0$). The trivial solution to this equation is to start *field neutral* by microscopically placing a charge-compensating amount of free electrons on the same position as according ions.

Fully Ionized Ions

For fully ionized ions, just use `ManipulateDerive` in *speciesInitialization.param* and derive macro-electrons $1:1$ from macro-ions but increase their weighting by $1:Z$ of the ion.

```
using InitPipeline = bmpl::vector<
    /* density profile from density.param and
     *     start position from particle.param */
    CreateDensity<
        densityProfiles::YourSelectedProfile,
        startPosition::YourStartPosition,
        Carbon
    >,
    /* create a macro electron for each macro carbon but increase its
     *     weighting by the ion's proton number so it represents all its
     *     electrons after an instantanous ionization */
    ManipulateDerive<
        manipulators::ProtonTimesWeighting,
        Carbon,
        Electrons
    >
>;
```

If the `Carbon` species in this example has an attribute `boundElectrons` (optional, see *speciesAttributes.param and speciesDefinition.param*) and its value is not manipulated the default value is used (zero bound electrons, fully ionized). If the attribute `boundElectrons` is not added to the `Carbon` species the charge state is considered constant and taken from the `chargeRatio< ... >` particle flag.

Partly Ionized Ions

For partial pre-ionization, the *FoilLCT example* shows a detailed setup. First, define a functor that manipulates the number of bound electrons in *particle.param*, e.g. to *twice pre-ionized*.

```
#include "picongpu/particles/traits/GetAtomicNumbers.hpp"
// ...

namespace manipulators
{
    //! ionize ions twice
    struct TwiceIonizedImpl
    {
        template< typename T_Particle >
        DINLINE void operator()(
            T_Particle& particle
        )
        {
            constexpr float_X protonNumber =
                GetAtomicNumbers< T_Particle >::type::numberOfProtons;
            particle[ boundElectrons_ ] = protonNumber - float_X( 2. );
        }
    };

    //! definition of TwiceIonizedImpl manipulator
    using TwiceIonized = generic::Free< TwiceIonizedImpl >;

} // namespace manipulators
```

Then again in *speciesInitialization.param* set your initialization routines to:

```
using InitPipeline = bmpl::vector<
    /* density profile from density.param and
```

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```
     *     start position from particle.param */
    CreateDensity<
        densityProfiles::YourSelectedProfile,
        startPosition::YourStartPosition,
        Carbon
    >,
    /* partially pre-ionize the carbons by manipulating the carbon's
     *     `boundElectrons` attribute,
     *     functor defined in particle.param: set to C2+ */
    Manipulate<
        manipulators::TwiceIonized,
        Carbon
    >,
    /* does also manipulate the weighting x2 while deriving the electrons
     *     ("twice pre-ionized") since we set carbon as C2+ */
    ManipulateDerive<
        manipulators::binary::UnboundElectronsTimesWeighting,
        Carbon,
        Electrons
    >
>;
```

2.8.9 Probe Particles

Section author: Axel Huebl

Probe particles ("probes") can be used to record field quantities at selected positions over time.

As a geometric data-reduction technique, analyzing the discrete, regular field of a particle-in-cell simulation only at selected points over time can greatly reduce the need for I/O. Such particles are often arranged at isolated points, regularly as along lines, in planes or in any other user-defined manner.

Probe particles are usually neutral, non-interacting test particles that are statically placed in the simulation or co-moving with along pre-defined path. Self-consistently interacting particles are usually called *tracer particles*.

Workflow

- `speciesDefinition.param`: create a stationary probe species, add `probeE` and `probeB` attributes to it for storing interpolated fields

```
using ParticleFlagsProbes = MakeSeq_t<
    particlePusher< particles::pusher::Probe >,
    shape< UsedParticleShape >,
    interpolation< UsedField2Particle >
>;

using Probes = Particles<
    PMACC_CSTRING( "probe" ),
    ParticleFlagsProbes,
    MakeSeq_t<
        position< position_pic >,
        probeB,
        probeE
    >
>;
```

and add it to `VectorAllSpecies`:

```
using VectorAllSpecies = MakeSeq_t<
    Probes,
    // ...
>;
```

- `density.param`: select in which cell a probe particle shall be placed, e.g. in each 4th cell per direction:

```
// put probe particles every 4th cell in X, Y(, Z)
using ProbeEveryFourthCell = EveryNthCellImpl<
    mCT::UInt32<
        4,
        4,
        4
    >
>;
```

- `particle.param`: initialize the individual probe particles in-cell, e.g. always in the left-lower corner and only one per selected cell

```
CONST_VECTOR(
    float_X,
    3,
    InCellOffset,
    /* each x, y, z in-cell position component
     * in range [0.0, 1.0) */
    0.0,
    0.0,
    0.0
);
struct OnePositionParameter
{
    static constexpr uint32_t numParticlesPerCell = 1u;
    const InCellOffset_t inCellOffset;
};

using OnePosition = OnePositionImpl< OnePositionParameter >;
```

- `speciesInitialization.param`: initialize particles for the probe just as with regular particles

```
using InitPipeline = bmpl::vector<
    // ... ,
    CreateDensity<
        densityProfiles::ProbeEveryFourthCell,
        startPosition::OnePosition,
        Probes
    >
>;
```

- `fileOutput.param`: make sure the the probe particles are part of `FileOutputParticles`

```
// either all via VectorAllSpecies or just select
using FileOutputParticles = MakeSeq_t< Probes >;
```

Known Limitations

Note: currently, only the electric field $\vec{E}$ and the magnetic field $\vec{B}$ can be recorded

Note: we currently do not support time averaging

Warning: If the probe particles are dumped in the file output, the instantaneous fields they recorded will be one time step behind the last field update (since our runOneStep pushed the particles first and then calls the field solver). Adding the attributes `probeE` or `probeB` to a species will increase the particle memory footprint only for the corresponding species by `3 * sizeof(float_X)` byte per attribute and particle.

2.8.10 Tracer Particles

Section author: Axel Huebl

Tracer particles are like *probe particles*, but interact self-consistenly with the simulation. They are usually used to visualize *representative* particle trajectories of a larger distribution.

In PIConGPU each species can be a tracer particle species, which allows tracking fields along the particle trajectory.

Workflow

- `speciesDefinition.param`:

Add the particle attribute `particleId` to your species to give each particle a unique id. The id is optional and only required if the particle should be tracked over time. Adding `probeE` creates a tracer species stores the interpolated electric field seen by the tracer particle.

```
using ParticleFlagsTracerElectrons = MakeSeq_t<
    particlePusher< particles::pusher::Boris >,
    shape< UsedParticleShape >,
    interpolation< UsedField2Particle >,
    currentSolver::Esirkepov<UsedParticleCurrentSolver>
>;

using TracerElectron = Particles<
    PMACC_CSTRING( "e_tracer" ),
    ParticleFlagsTracerElectrons,
    MakeSeq_t<
        position< position_pic >,
        momentum,
        weighting,
        particleId,
        probeE
    >
>;
```

and add it to `VectorAllSpecies`:

```
using VectorAllSpecies = MakeSeq_t<
    TracerElectron,
    // ...
>;
```

- create tracer particles by either
  - `speciesInitialization.param`: initializing a low percentage of your initial density inside this species or
  - `speciesInitialization.param`: assigning the target (electron) species of an ion's ionization routine to the tracer species or

  - `speciesInitialization.param`: moving some particles of an already initialized species to the tracer species (upcoming)
- `fileOutput.param`: make sure the the tracer particles are part of `FileOutputParticles`

```
// either all via VectorAllSpecies or just select
using FileOutputParticles = MakeSeq_t< TracerElectron >;
```

The electron tracer species is equivalent to normal electrons, the initial density distribution can be configured in *speciesInitialization.param*.

Known Limitations

- currently, only the electric field $\vec{E}$ and the magnetic field $\vec{B}$ can be recorded
- we currently do not support time averaging

2.8.11 Particle Filters

Section author: Axel Huebl, Sergei Bastrakov

A common task in both modeling, initializing and in situ processing (output) is the selection of particles of a particle species by attributes. PIConGPU implements such selections as *particle filters*.

Particle filters are simple mappings assigning each particle of a species either `true` or `false` (ignore / filter out). These filters can be defined in *particleFilters.param*.

Example

Let us select particles with momentum vector within a cone with an opening angle of five degrees (pinhole):

```
namespace picongpu
{
namespace particles
{
namespace filter
{
    struct FunctorParticlesForwardPinhole
    {
        static constexpr char const * name = "forwardPinhole";

        template< typename T_Particle >
        HDINLINE bool operator()(
            T_Particle const & particle
        )
        {
            bool result = false;
            float3_X const mom = particle[ momentum_ ];
            float_X const absMom = math::abs( mom );

            if( absMom > float_X( 0. ) )
            {
                /* place detector in y direction, "infinite distance" to target,
                 * and five degree opening angle
                 */
                constexpr float_X openingAngle = 5.0 * PI / 180.;
                float_X const dotP = mom.y() / absMom;
                float_X const degForw = math::acos( dotP );

                if( math::abs( degForw ) <= openingAngle * float_X( 0.5 ) )
```

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```
                    result = true;
            }
            return result;
        }
    };
    using ParticlesForwardPinhole = generic::Free<
       FunctorParticlesForwardPinhole
    >;
```

and add `ParticlesForwardPinhole` to the `AllParticleFilters` list:

```
    using AllParticleFilters = MakeSeq_t<
        All,
        ParticlesForwardPinhole
    >;

} // namespace filter
} // namespace particles
} // namespace picongpu
```

Filtering Based on Global Position

A particle only stores its relative position inside the cell. Thus, with a simple filter like one shown above, it is not possible to get global position of a particle. However, there are helper wrapper filters that provide such information in addition to the particle data.

For a special case of slicing along one axis this is a simple existing filter that only needs to be parametrized:

```
namespace picongpu
{
namespace particles
{
namespace filter
{
    namespace detail
    {
        //! Parameters to be used with RelativeGlobalDomainPosition, change the␣
↪values inside
        struct SliceParam
        {
            // Lower bound in relative coordinates: global domain is [0.0, 1.0]
            static constexpr float_X lowerBound = 0.55_X;

            // Upper bound in relative coordinates
            static constexpr float_X upperBound = 0.6_X;

            // Axis: x = 0; y= 1; z = 2
            static constexpr uint32_t dimension = 0;

            // Text name of the filter, will be used in .cfg file
            static constexpr char const* name = "slice";
        };

        //! Use the existing RelativeGlobalDomainPosition filter with our␣
↪parameters
        using Slice = RelativeGlobalDomainPosition<SliceParam>;
    }
```

and add `detail::Slice` to the `AllParticleFilters` list:

```
    using AllParticleFilters = MakeSeq_t<
        All,
        detail::Slice
    >;

} // namespace filter
} // namespace particles
} // namespace picongpu
```

For a more general case of filtering based on cell index (possibly combined with other particle properties) use the following pattern:

```
namespace picongpu
{
namespace particles
{
namespace filter
{
    namespace detail
    {
        struct AreaFilter
        {
            static constexpr char const* name = "areaFilter";

            template<typename T_Particle>
            HDINLINE bool operator()(
                DataSpace<simDim> const totalCellOffset,
                T_Particle const & particle
            )
            {
                /* Here totalCellOffset is the cell index of the particle in the␣
↪total coordinate system.
                 * So we can define conditions based on both cell index and other␣
↪particle data.
                 */
                return (totalCellOffset.x() >= 10) && (particle[momentum_].x() < 0.
↪0_X);
            }
        };

        //! Wrap AreaFilter so that it fits the general filter interface
        using Area = generic::FreeTotalCellOffset<AreaFilter>;
    }
```

and add `detail::Area` to the `AllParticleFilters` list:

```
    using AllParticleFilters = MakeSeq_t<
        All,
        detail::Area
    >;

} // namespace filter
} // namespace particles
} // namespace picongpu
```

Limiting Filters to Eligible Species

Besides *the list of pre-defined filters* with parametrization, users can also define generic, "free" implementations as shown above. All filters are added to `AllParticleFilters` and then *combined with all available species* from `VectorAllSpecies` (see *speciesDefinition.param*).

In the case of user-defined free filters we can now check if each species in `VectorAllSpecies` fulfills the requirements of the filter. That means: if one accesses specific *attributes* or *flags* of a species in a filter, they must exist or will lead to a compile error.

As an example, *probe particles* usually do not need a `momentum` attribute which would be used for an energy filter. So they should be ignored from compilation when combining filters with particle species.

In order to exclude all species that have no `momentum` attribute from the `ParticlesForwardPinhole` filter, specialize the C++ trait `SpeciesEligibleForSolver`. This trait is implemented to be checked during compile time when combining filters with species:

```
// ...

} // namespace filter

namespace traits
{
    template<
        typename T_Species
    >
    struct SpeciesEligibleForSolver<
        T_Species,
        filter::ParticlesForwardPinhole
    >
    {
        using type = typename pmacc::traits::HasIdentifiers<
            typename T_Species::FrameType,
            MakeSeq_t< momentum >
        >::type;
    };
} // namespace traits
} // namespace particles
} // namespace picongpu
```

CHAPTER

THREE

MODELS

3.1 The Particle-in-Cell Algorithm

Section author: Axel Huebl, Klaus Steiniger

Please also refer to the textbooks [BirdsallLangdon], [HockneyEastwood], our *latest paper on PIConGPU* and the works in [Huebl2014] and [Huebl2019] .

3.1.1 System of Equations

$$
\begin{aligned}
\nabla \cdot \mathbf{E} &= \frac{1}{\varepsilon_0} \sum_s \rho_s \\
\nabla \cdot \mathbf{B} &= 0 \\
\nabla \times \mathbf{E} &= -\frac{\partial \mathbf{B}}{\partial t} \\
\nabla \times \mathbf{B} &= \mu_0 \left(\sum_s \mathbf{J}_s + \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right)
\end{aligned}
$$

for multiple particle species s. $\mathbf{E}(t)$ represents the electric, $\mathbf{B}(t)$ the magnetic, ρ_s the charge density and $\mathbf{J}_s(t)$ the current density field.

Except for normalization of constants, PIConGPU implements the governing equations in SI units.

3.1.2 Relativistic Plasma Physics

The 3D3V particle-in-cell method is used to describe many-body systems such as a plasmas. It approximates the Vlasov–Maxwell–Equation

$$
\partial_t f_s(\mathbf{x}, \mathbf{v}, t) + \mathbf{v} \cdot \nabla_x f_s(\mathbf{x}, \mathbf{v}, t) + \frac{q_s}{m_s} \left[\mathbf{E}(\mathbf{x}, t) + \mathbf{v} \times \mathbf{B}(\mathbf{x}, t) \right] \cdot \nabla_v f_s(\mathbf{x}, \mathbf{v}, t) = 0 \tag{3.1}
$$

with f_s as the distribution function of a particle species s, $\mathbf{x}$, $\mathbf{v}$, t as position, velocity and time and $\frac{q_s}{m_s}$ the charge to mass-ratio of a species. The momentum is related to the velocity by $\mathbf{p} = \gamma m_s \mathbf{v}$.

The equations of motion are given by the Lorentz force as

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t} \mathbf{V_s}(t) &= \frac{q_s}{m_s} \left[\mathbf{E}(\mathbf{X_s}(t), t) + \mathbf{V_s}(t) \times \mathbf{B}(\mathbf{X_s}(t), t) \right] \\
\frac{\mathrm{d}}{\mathrm{d}t} \mathbf{X_s}(t) &= \mathbf{V_s}(t).
\end{aligned}
$$

Attention: TODO: write proper relativistic form

$\mathbf{X}_s = (\mathbf{x}_1, \mathbf{x}_2, ...)_s$ and $\mathbf{V}_s = (\mathbf{v}_1, \mathbf{v}_2, ...)_s$ are vectors of *marker* positions and velocities, respectively, which describe the ensemble of particles belonging to species s.

Note: Particles in a particle species can have different charge states in PIConGPU. In the general case, $\frac{q_s}{m_s}$ is not required to be constant per particle species.

3.1.3 Electro-Magnetic PIC Method

Fields such as $\mathbf{E}(t), \mathbf{B}(t)$ and $\mathbf{J}(t)$ are discretized on a regular mesh in Eulerian frame of reference (see [EulerLagrangeFrameOfReference]). See *section Finite-Difference Time-Domain Method* describing how Maxwell's equations are discretized on a mesh in PIConGPU.

The distribution of **Particles** is described by the distribution function $f_s(\mathbf{x}, \mathbf{v}, t)$. This distribution function is sampled by *markers*, which are commonly referred to as *macroparticles*. These markers represent blobs of incompressible phase fluid moving in phase space. The temporal evolution of the distribution function is simulated by advancing the markers over time according to the Vlasov–Maxwell–Equation in Lagrangian frame (see eq. (3.1) and [EulerLagrangeFrameOfReference]). A marker has a finite-size and a velocity, such that it can be regarded as a cloud of particles, whose center of mass is the marker's position and whose mean velocity is the marker's velocity. The cloud shape $S^n(x)$ of order n of a marker describes its charge density distribution. See *section Hierarchy of Charge Assignment Schemes* for a list of available marker shapes in PIConGPU.

3.1.4 References

3.2 Finite-Difference Time-Domain Method

Section author: Klaus Steiniger, Jakob Trojok

For the discretization of Maxwell's equations on a mesh in PIConGPU, only the equations

$$\frac{1}{c^2}\frac{\partial}{\partial t}\vec{E} = \nabla \times \vec{B} - \mu_0 \vec{J}$$
$$\frac{\partial}{\partial t}\vec{B} = -\nabla \times \vec{E}$$

are solved. This becomes possible, first, by correctly solving Gauss's law $\nabla \cdot \vec{E} = \frac{1}{\varepsilon_0}\sum_s \rho_s$ using Esirkepov's current deposition method [Esirkepov2001] (or variants thereof) which solve the discretized continuity equation exactly. Second, by assuming that the initially given electric and magnetic field satisfy Gauss' laws. Starting simulations in an initially charge free and magnetic-divergence-free space, i.e.

$$\nabla \cdot \vec{E} = 0$$
$$\nabla \cdot \vec{B} = 0$$

is standard.

3.2.1 Discretization on a staggered mesh

In the Finite-Difference Time-Domain method, above Maxwell's equations are discretized by replacing the partial space and time derivatives with centered finite differences. For example, the partial space derivative along x of a scalar field u at position (i, j, k) and time step n becomes

$$\partial_x u(i\Delta x, j\Delta y, k\Delta z, n\Delta t) = \frac{u^n_{i+1/2,j,k} - u^n_{i-1/2,j,k}}{\Delta x}$$

and the temporal derivative becomes

$$\partial_t u(i\Delta x, j\Delta y, k\Delta z, n\Delta t) = \frac{u^{n+1/2}_{i,j,k} - u^{n-1/2}_{i,j,k}}{\Delta t},$$

when replacing with the lowest order central differences. Note, with this leapfrog discretization or staggering, derivatives of field quantities are calculated at positions between positions where the field quantities are known.

The above discretization uses one neighbor to each side from the point where the derivative is calculated yielding a second order accurate approximation of the derivative. Using more neighbors for the approximation of the spatial derivative is possible in PIConGPU and reduces the discretization error. Which is to say that the order of the method is increased. The error order scales with twice the number of neighbors M used to approximate the derivative. The arbitrary order finite difference of order $2M$ reads

$$\partial_x u(i\Delta x, j\Delta y, k\Delta z, n\Delta t) = \sum_{l=1/2}^{M-1/2} \left[g_l^{2M} \frac{u^n_{i+l,j,k} - u^n_{i-l,j,k}}{\Delta x} \right], \text{where}$$

$$g_l^{2M} = \frac{(-1)^{l-1/2}}{2l^2} \frac{((2M-1)!!)^2}{(2M-1-2l)!!(2M-1+2l)!!}$$

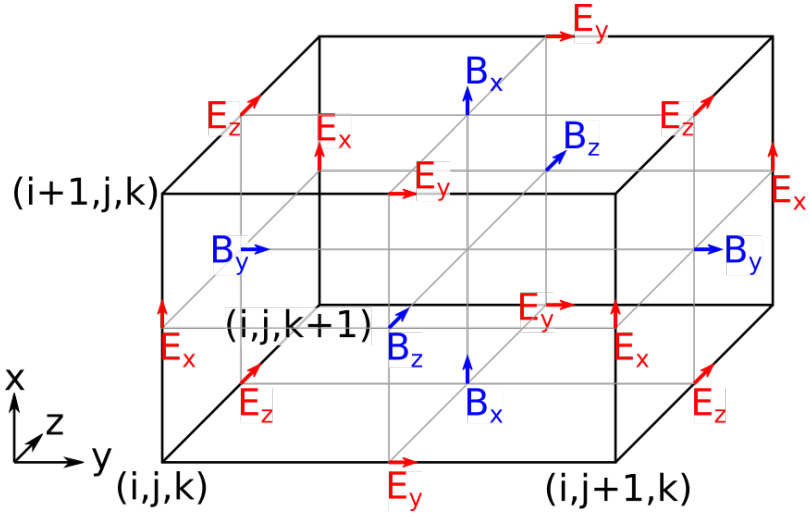
with $l = -M+1/2, -M+1+1/2, ..., -1/2, 1/2, ..., M-1/2$ [Ghrist2000]. A recurrence relation for the weights exists,

$$g_l^{2M} = (-1)\frac{(l-1)^2}{l^2}\frac{(2M+1-2l)}{(2M-1+2l)} g_{l-1}^{2M}$$

$$g_{\frac{1}{2}}^{2M} = \frac{16^{1-M}}{M}\left(\frac{(2M-1)!}{[(M-1)!]^2}\right)^2$$

3.2.2 Maxwell's equations on the mesh

When discretizing on the mesh with centered finite differences, the spatial positions of field components need to be chosen such that a field component, whose **temporal derivative** is calculated on the left hand side of a Maxwell equation, is spatially positioned between the two field components whose **spatial derivative** is evaluated on the right hand side of the respective Maxwell equation. In this way, the spatial points where a left hand side temporal derivative of a field is evaluate lies exactly at the position where the spatial derivative of the right hand side fields is calculated. The following image visualizes the arrangement of field components in PIConGPU.



Component-wise and using second order finite differences for the derivative approximation, Maxwell's equations

read in PIConGPU

$$
\begin{aligned}
\frac{E_x|^{n+1}_{i+1/2,j,k} - E_x|^{n}_{i+1/2,j,k}}{c^2\Delta t} =& \frac{B_z|^{n+1/2}_{i+1/2,j+1/2,k} - B_z|^{n+1/2}_{i+1/2,j-1/2,k}}{\Delta y} \\
& - \frac{B_y|^{n+1/2}_{i+1/2,j,k+1/2} - B_y|^{n+1/2}_{i+1/2,j,k-1/2}}{\Delta z} - \mu_0 J_x|^{n+1/2}_{i+1/2,j,k} \\
\frac{E_y|^{n+1}_{i,j+1/2,k} - E_y|^{n}_{i,j+1/2,k}}{c^2\Delta t} =& \frac{B_x|^{n+1/2}_{i,j+1/2,k+1/2} - B_x|^{n+1/2}_{i,j+1/2,k-1/2}}{\Delta z} \\
& - \frac{B_z|^{n+1/2}_{i+1/2,j+1/2,k} - B_z|^{n+1/2}_{i-1/2,j+1/2,k}}{\Delta x} - \mu_0 J_y|^{n+1/2}_{i,j+1/2,k} \\
\frac{E_z|^{n+1}_{i,j,k+1/2} - E_z|^{n}_{i,j,k+1/2}}{c^2\Delta t} =& \frac{B_y|^{n+1/2}_{i+1/2,j,k+1/2} - B_y|^{n+1/2}_{i-1/2,j,k+1/2}}{\Delta x} \\
& - \frac{B_x|^{n+1/2}_{i,j+1/2,k+1/2} - B_x|^{n+1/2}_{i,j-1/2,k+1/2}}{\Delta y} - \mu_0 J_z|^{n+1/2}_{i,j,k+1/2} \\
\frac{B_x|^{n+3/2}_{i,j+1/2,k+1/2} - B_x|^{n+1/2}_{i,j+1/2,k+1/2}}{\Delta t} =& \frac{E_y|^{n+1}_{i,j+1/2,k+1} - E_y|^{n+1}_{i,j+1/2,k}}{\Delta z} - \frac{E_z|^{n+1}_{i,j+1,k+1/2} - E_z|^{n+1}_{i,j,k+1/2}}{\Delta y} \\
\frac{B_y|^{n+3/2}_{i+1/2,j,k+1/2} - B_y|^{n+1/2}_{i+1/2,j,k+1/2}}{\Delta t} =& \frac{E_z|^{n+1}_{i+1,j,k+1/2} - E_z|^{n+1}_{i,j,k+1/2}}{\Delta x} - \frac{E_x|^{n+1}_{i+1/2,j,k+1} - E_x|^{n+1}_{i+1/2,j,k}}{\Delta z} \\
\frac{B_z|^{n+3/2}_{i+1/2,j+1/2,k} - B_z|^{n+1/2}_{i+1/2,j+1/2,k}}{\Delta t} =& \frac{E_x|^{n+1}_{i+1/2,j+1,k} - E_x|^{n+1}_{i+1/2,j,k}}{\Delta y} - \frac{E_y|^{n+1}_{i+1,j+1/2,k} - E_y|^{n+1}_{i,j+1/2,k}}{\Delta x}
\end{aligned}
$$

As can be seen from these equations, the components of the source current are located at the respective components of the electric field. Following Gauss's law, the charge density is located at the cell corner.

Using Esirkepov's notation for the discretized differential operators,

$$
\begin{aligned}
\nabla^+ u_{i,j,k} &= \left(\frac{u_{i+1,j,k} - u_{i,j,k}}{\Delta x}, \frac{u_{i,j+1,k} - u_{i,j,k}}{\Delta y} \frac{u_{i,j,k+1} - u_{i,j,k}}{\Delta z} \right) \\
\nabla^- u_{i,j,k} &= \left(\frac{u_{i,j,k} - u_{i-1,j,k}}{\Delta x}, \frac{u_{i,j,k} - u_{i,j-1,k}}{\Delta y} \frac{u_{i,j,k} - u_{i,j,k-1}}{\Delta z} \right) ,
\end{aligned}
$$

the shorthand notation for the discretized Maxwell equations in PIConGPU reads

$$
\begin{aligned}
\frac{\vec{E}|^{n+1} - \vec{E}|^{n}}{c^2\Delta t} &= \nabla^- \times \vec{B}|^{n+1/2} - \mu_0 \vec{J}|^{n+1/2} \\
\frac{\vec{B}|^{n+3/2} - \vec{B}|^{n+1/2}}{\Delta t} &= -\nabla^+ \times \vec{E}|^{n+1} \\
\nabla^- \cdot \vec{E}|^{n+1} &= \rho|^{n+1} \\
\nabla^+ \cdot \vec{B}|^{n+3/2} &= 0 ,
\end{aligned}
$$

with initial conditions

$$
\begin{aligned}
\nabla^- \cdot \vec{E} &= 0 \\
\nabla^+ \cdot \vec{B} &= 0 .
\end{aligned}
$$

The components $E_x|_{1/2,0,0} = E_y|_{0,1/2,0} = E_z|_{0,0,1/2} = B_x|_{I,J+1/2,K+1/2} = B_y|_{I+1/2,J,K+1/2} = B_z|_{I+1/2,J+1/2,K} = 0$ for all times when using absorbing boundary conditions. Here, I, J, K are the maximum values of i, j, k defining the total mesh size.

Note, in PIConGPU the $\vec{B}$-field update is split in two updates of half the time step, e.g.

$$
\frac{B_x|^{n+1}_{i,j+1/2,k+1/2} - B_x|^{n+1/2}_{i,j+1/2,k+1/2}}{\Delta t/2} = \frac{E_y|^{n+1}_{i,j+1/2,k+1} - E_y|^{n+1}_{i,j+1/2,k}}{\Delta z} - \frac{E_z|^{n+1}_{i,j+1,k+1/2} - E_z|^{n+1}_{i,j,k+1/2}}{\Delta y}
$$

and

$$\frac{B_x|_{i,j+1/2,k+1/2}^{n+3/2} - B_x|_{i,j+1/2,k+1/2}^{n+1}}{\Delta t/2} = \frac{E_y|_{i,j+1/2,k+1}^{n+1} - E_y|_{i,j+1/2,k}^{n+1}}{\Delta z} - \frac{E_z|_{i,j+1,k+1/2}^{n+1} - E_z|_{i,j,k+1/2}^{n+1}}{\Delta y}$$

for the B_x component, where the second half of the update is performed at the beginning of the next time step such that the electric and magnetic field are known at equal time in the particle pusher and at the end of a time step.

3.2.3 Dispersion relation of light waves on a mesh

The dispersion relation of a wave relates its oscillation period in time T to its oscillation wavelength λ, i.e. its angular frequency $\omega = \frac{2\pi}{T}$ to wave vector $\vec{k} = \frac{2\pi}{\lambda}\vec{e}_k$. For an electromagnetic wave in vacuum,

$$\left[\frac{\omega}{c}\right]^2 = k_x^2 + k_y^2 + k_z^2 \,.$$

However, on a 3D mesh, with arbitrary order finite differences for the spatial derivatives, the dispersion relation becomes

$$\left[\frac{1}{c\Delta t}\sin\left(\frac{\omega\Delta t}{2}\right)\right]^2 = \left[\sum_{l=1/2}^{M-1/2} g_l^{2M}\frac{\sin(\tilde{k}_x l\Delta x)}{\Delta x}\right]^2 + \left[\sum_{l=1/2}^{M-1/2} g_l^{2M}\frac{\sin(\tilde{k}_y l\Delta y)}{\Delta y}\right]^2 + \left[\sum_{l=1/2}^{M-1/2} g_l^{2M}\frac{\sin(\tilde{k}_z l\Delta z)}{\Delta z}\right]^2$$

where $\tilde{k}_x$, $\tilde{k}_y$, and $\tilde{k}_z$ are the wave vector components on the mesh in x, y, and z direction, respectively. As is obvious from the relation, the numerical wave vector will be different from the real world wave vector for a given frequency ω due to discretization.

Dispersion Relation for Yee's Method

Yee's method [Yee1966] uses second order finite differences for the approximation of spatial derivatives. The corresponding dispersion relation reads

$$\left[\frac{1}{c\Delta t}\sin\left(\frac{\omega\Delta t}{2}\right)\right]^2 = \left[\frac{1}{\Delta x}\sin\left(\frac{\tilde{k}_x\Delta x}{2}\right)\right]^2 + \left[\frac{1}{\Delta y}\sin\left(\frac{\tilde{k}_y\Delta y}{2}\right)\right]^2 + \left[\frac{1}{\Delta z}\sin\left(\frac{\tilde{k}_z\Delta z}{2}\right)\right]^2 .$$

Obviously, this is a special case of the general dispersion relation, where $M = 1$.

Solving for a wave's numerical frequency ω in dependence on its wave vector $\vec{\tilde{k}} = (\tilde{k}\cos\phi\sin\theta, \tilde{k}\sin\phi\sin\theta, \tilde{k}\cos\theta)$ (spherical coordinates),

$$\omega = \frac{2}{\Delta t}\arcsin\xi \,, \text{ where } \xi_{\max} = c\Delta t\sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}$$

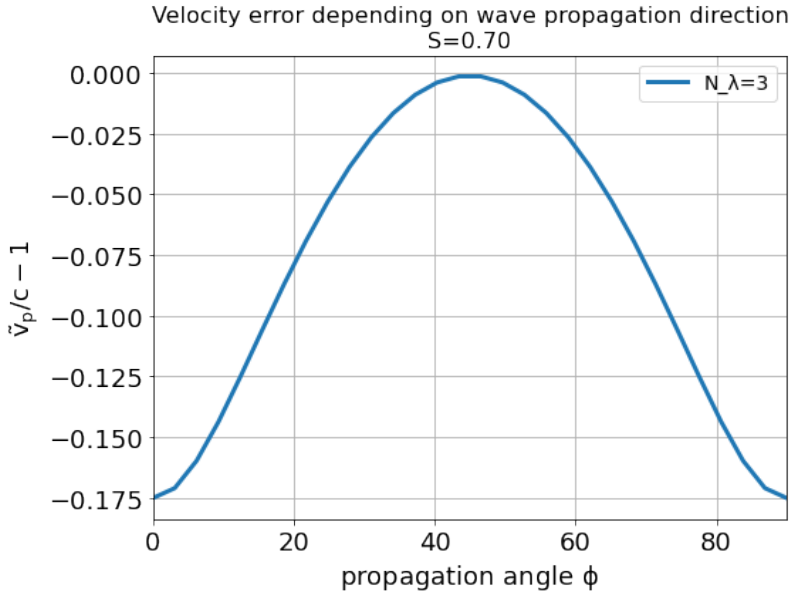
reveals two important properties of the field solver. (The 2D version is obtained by letting $\Delta z \to \infty$.)

First, only within the range $\xi_{\max} \leq 1$ the field solver operates stable. This gives the *Courant-Friedrichs-Lewy* stability condition relating time step to mesh spacing

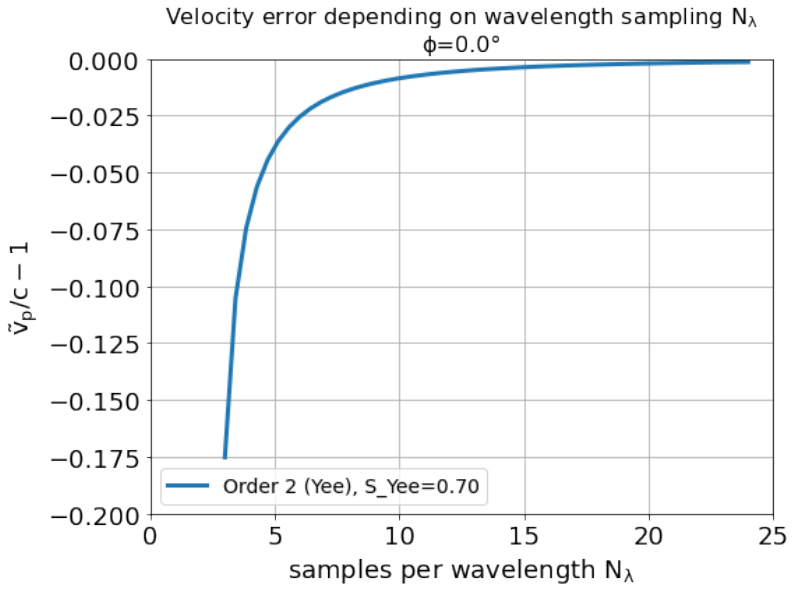
$$c\Delta t < \frac{1}{\sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}}$$

Typically, $\xi_{\max} = 0.995$ is chosen. Outside this stability region, the frequency ω corresponding to a certain wave vector becomes imaginary, meaning that wave amplitudes can be nonphysical exponentially amplified [Taflove2005].

Second, there exists a purely numerical anisotropy in a wave's phase velocity $\tilde{v}_p = \omega/\tilde{k}$ (speed of electromagnetic wave propagation) depending on its propagation direction ϕ, as depicted in the following figure



assuming square cells $\Delta x = \Delta y = \Delta$ and where $S = c\Delta t/\Delta$, $N_\lambda = \lambda/\Delta$. That is, for the chosen sampling of three samples per wavelength λ, the phase velocities along a cell edge and a cell diagonal differ by approximately 20%. The velocity error is largest for propagation along the edge. The phase velocity error can be significantly reduced by increasing the sampling, as visualized in the following figure by the scaling of the velocity error with wavelength sampling for propagation along the cell edge



Another conclusion from this figure is, that a short-pulse laser with a large bandwidth will suffer from severe dispersion if the sampling is bad. In the extreme case where a wavelength is not even sampled twice on the mesh, its field is exponentially damped [Taflove2005].

Given that most simulations employ short-pulse lasers propagating along the y-axis and featuring a large bandwidth, the resolution of the laser wavelength should be a lot better than in the example, e.g. $N_\lambda = 24$, to reduce errors due to numerical dispersion.

Note, the reduced phase velocity of light can further cause the emission of numerical Cherenkov radiation by fast charged particles in the simulation [Lehe2012]. The largest emitted wavelength equals the wavelength whose phase velocity is as slow as the particle's velocity, provided it is resolved at least twice on the mesh.

Dispersion Relation for Arbitrary Order Finite Differences

Solving the higher order dispersion relation for the angular frequency yields:

$$\omega = \frac{2}{\Delta t} \arcsin \xi \text{ , where } \xi_{\max} = c\Delta t \left[\sum_{l=1/2}^{M-1/2} (-1)^{l-\frac{1}{2}} g_l^{2M} \right] \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}$$

The equation is structurally the same as for Yee's method, but contains the alternating sum of the weighting coefficients of the spatial derivative. Again, Yee's Formula is the special case where $M = 1$. For the solver to be stable, $\xi_{\max} < 1$ is required as before. Thus the stability condition reads

$$c\Delta t < \frac{1}{\left[\sum_{l=1/2}^{M-1/2} (-1)^{l-\frac{1}{2}} g_l^{2M} \right] \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}}$$

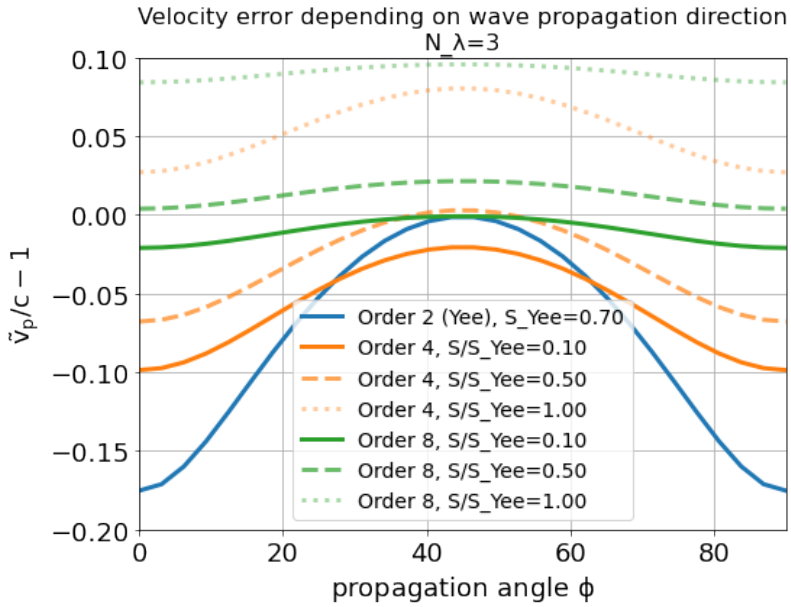
As explained for Yee's method, $\xi_{\max} = 0.995$ is normally chosen and not meeting the stability condition can lead to nonphysical exponential wave amplification.

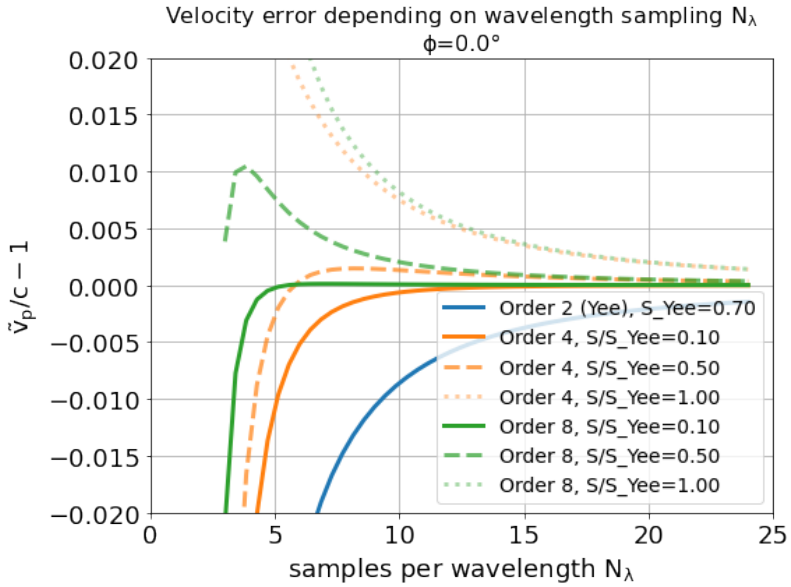
Sample values for the additional factor $\left[\sum_{l=1/2}^{M-1/2} (-1)^{l-\frac{1}{2}} g_l^{2M} \right]$ appearing in the AOFDTD stability condition compared to Yee's method, are

Number of neighbors M	Value of additional factor $\sum(-1)^{l-\frac{1}{2}} g_l^{2M}$
1	1.0
2	1.166667
3	1.241667
4	1.286310
5	1.316691
6	1.339064
7	1.356416
8	1.370381

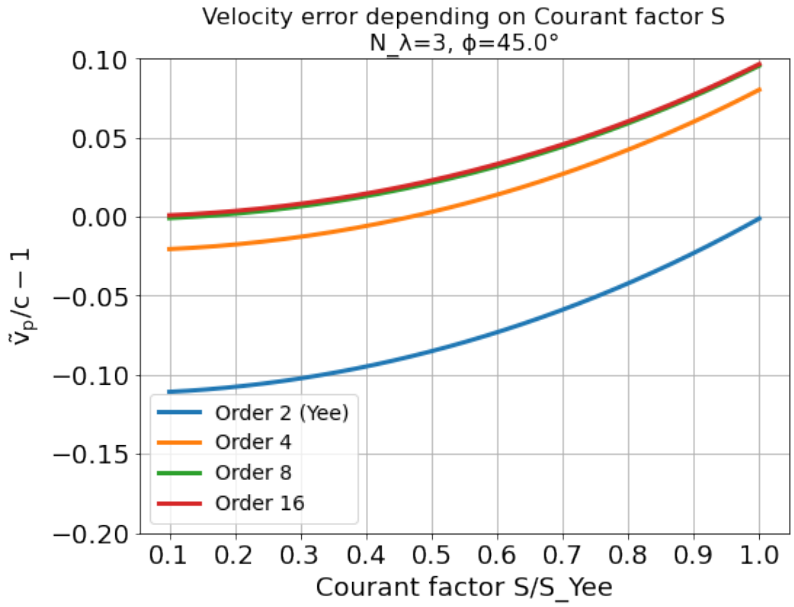
which implies a reduction of the usable time step Δt by the given factor if more than one neighbor is used.

Regarding the numerical anisotropy of the phase velocity, using higher order finite differences for the approximation of spatial derivatives significantly improves the dispersion properties of the solver. Most notably, the velocity anisotropy reduces and the dependence of phase velocity on sampling reduces, too. Yet higher order solvers still feature dispersion. As shown in the following picture, its effect is, however, not reduction of phase velocity but increase of phase velocity beyond the physical vacuum speed of light. But this can be tweaked by reducing the time step relative to the limit set by the stability criterion.





Note, it is generally not a good idea to reduce the time step in Yee's method significantly below the stability criterion as this increases the absolute phase velocity error. See the following figure,



from which the optimum Courant factor $S = c\Delta t/\Delta$ can be read off for a 2D, square mesh, too.

An important conclusion from the above figures showing velocity error over sampling is, that a higher order solver, with a larger mesh spacing and a smaller time step than given by the above stability limit, produces physically more accurate results than the standard Yee solver operating with smaller mesh spacing and a time step close to the stability limit.

That is, it can be beneficial not only in terms of **physical accuracy**, but also in terms of **memory complexity** and **time to solution**, to chose a higher order solver with lower spatial resolution and increased time sampling relative to the stability limit. Memory complexity scales with number of cells N_{cells} required to sample a given volume N_{cells}^d, where $d = 2, 3$ is the dimension of the simulation domain, which decreases for larger cells. Time to solution scales with the time step and this can be larger with solvers of higher order compared to the Yee solver with comparable dispersion properties (which requires a smaller cell size than the arbitrary order solver) since the time step is limited by the stability condition which scales with cell size. Since the cell size can be larger for arbitrary order solvers, the respective time step limit given by the stability condition is larger and operating with a time step ten times smaller than the limit might still result in a larger step than those of the comparable Yee solver. Finally, physical accuracy is increased by the reduction of the impact of dispersion effects.

3.2.4 Usage

The field solver can be chosen and configured in *fieldSolver.param*.

3.2.5 References

3.3 Hierarchy of Charge Assignment Schemes

Section author: Klaus Steiniger

In PIConGPU, the cloud shapes $S^n(x)$ are pre-integrated to *assignment functions* $W^n(x)$.

$$W^n(x) = \Pi(x) * S^n(x) = \int_{-\infty}^{+\infty} \Pi(x') S^n(x' - x) dx' \,, \text{ where } \Pi(x) = \begin{cases} 0 & |x| \frac{1}{2} \\ \frac{1}{2} & |x| = \frac{1}{2} \\ 1 & |x| \frac{1}{2} \end{cases}$$

is the top-hat function and $*$ the convolution.

Evaluating the assignment functions at mesh points directly provides the fraction of charge from the marker assigned to that point.

The assignment functions are implemented as B-splines. The zeroth order assignment function W^0 is the top-hat function Π. It represents charge assignment to the nearest mesh point only, resulting in a stepwise charge density distribution. Therefore, it should not be used. The assignment function of order n is generated by convolution of the assignment function of order $n-1$ with the top-hat function

$$W^n(x) = W^{n-1}(x) * \Pi(x) = \int_{-\infty}^{+\infty} W^{n-1}(x')\Pi(x'-x)dx' \,.$$

The three dimensional assignment function is a multiplicative union of B-splines $W^n(x,y,z) = W^n(x)W^n(y)W^n(z)$.

PIConGPU implements these up to order $n = 4$. The naming scheme follows [HockneyEastwood], tab. 5-1, p. 144, where the name of a scheme is defined by the visual form of its cloud shape S.

Scheme	Order	Assignment function
NGP (nearest-grid-point)	0	stepwise
CIC (cloud-in-cell)	1	piecewise linear spline
TSC (triangular shaped cloud)	2	piecewise quadratic spline
PQS (piecewise quadratic cloud shape)	3	piecewise cubic spline
PCS (piecewise cubic cloud shape)	4	piecewise quartic spline

3.3.1 References

3.4 Landau-Lifschitz Radiation Reaction

Module author: Richard Pausch, Marija Vranic

To do

3.4.1 References

3.5 Field Ionization

Section author: Marco Garten

Module author: Marco Garten

Get started here https://github.com/ComputationalRadiationPhysics/picongpu/wiki/Ionization-in-PIConGPU

PIConGPU features an adaptable ionization framework for arbitrary and combinable ionization models.

Note: Most of the calculations and formulae in this section of the docs are done in the **Atomic Units (AU)** system.

$$\hbar = \mathrm{e} = m_\mathrm{e} = 1$$

Table 3.1: **Atomic Unit System**

AU	SI
length	$5.292 \cdot 10^{-11}\,\mathrm{m}$
time	$2.419 \cdot 10^{-17}\,\mathrm{s}$
energy	$4.360 \cdot 10^{-18}\,\mathrm{J}$ (= 27.21 eV = 1 Rydberg)
electrical field	$5.142 \cdot 10^{11}\,\frac{\mathrm{V}}{\mathrm{m}}$

3.5.1 Overview: Implemented Models

ionization regime	implemented model	reference
Multiphoton	None, yet	
Tunneling	• `Keldysh` • `ADKLinPol` • `ADKCircPol`	• [BauerMulser1999] • [DeloneKrainov] • [DeloneKrainov]
Barrier Suppression	• `BSI` • `BSIEffectiveZ` (R&D) • `BSIStarkShifted` (R&D)	• [MulserBauer2010] • [ClementiRaimondi1963] [ClementiRaimondi1967] • [BauerMulser1999]

Attention: Models marked with "(R&D)" are under *research and development* and should be used with care.

3.5.2 Ionization Current

In order to conserve energy, PIConGPU supports an ionization current to decrease the electric field according to the amount of energy lost to field ioniztion processes. The current for a single ion is

$$\mathbf{J}_{\text{ion}} = E_{\text{ion}} \frac{\mathbf{E}}{|\mathbf{E}|^2 \Delta t V_{\text{cell}}}$$

It is assigned to the grid according to the macroparticle shape. E_{ion} is the energy required to ionize the atom/ion, $\mathbf{E}$ is the electric field at the particle position and V_{cell} is the cell volume. This formula makes the assumption that the ejection energy of the electron is zero. See [Mulser]. The ionization current is accessible in *speciesDefinition.param*. To activate ionization current, set the second template of the ionization model to particles::ionization::current::EnergyConservation. By default the ionization current is deactivated.

3.5.3 Usage

Input for ionization models is defined in *speciesDefinition.param*, *ionizer.param and ionizationEnergies.param*.

3.5.4 Barrier Suppression Ionization

The so-called barrier-suppression ionization regime is reached for strong fields where the potential barrier binding an electron is completely suppressed.

3.5.5 Tunneling Ionization

Tunneling ionization describes the process during which an initially bound electron quantum-mechanically tunnels through a potential barrier of finite height.

Keldysh

$$\Gamma_{\text{K}} = \frac{(6\pi)^{1/2}}{2^{5/4}} E_{\text{ip}} \left(\frac{F}{(2E_{\text{ip}})^{3/2}} \right)^{1/2} \exp\left(-\frac{2\,(2E_{\text{ip}})^{3/2}}{3F} \right)$$

The Keldysh ionization rate has been implemented according to the equation (9) in [BauerMulser1999]. See also [Keldysh] for the original work.

Note: Assumptions:

- low field - perturbation theory
- $\omega_{\text{laser}} \ll E_{\text{ip}}$
- $F \ll F_{\text{BSI}}$
- tunneling is instantaneous

Ammosov-Delone-Krainov (ADK)

$$\Gamma_{\text{ADK}} = \underbrace{\sqrt{\frac{3n^{*3}F}{\pi Z^3}}}_{\text{lin. pol.}} \frac{FD^2}{8\pi Z} \exp\left(-\frac{2Z^3}{3n^{*3}F}\right) \tag{3.2}$$

$$D \equiv \left(\frac{4\mathrm{e}Z^3}{Fn^{*4}}\right)^{n^*} \qquad n^* \equiv \frac{Z}{\sqrt{2E_{\text{ip}}}} \tag{3.3}$$

We implemented equation (7) from [DeloneKrainov] which is a *simplified result assuming s-states* (since we have no atomic structure implemented, yet). Leaving out the pre-factor distinguishes `ADKCircPol` from `ADKLinPol`. `ADKLinPol` results from replacing an instantaneous field strength F by $F\cos(\omega t)$ and averaging over one laser period.

> **Attention:** Be aware that Z denotes the **residual ion charge** and not the proton number of the nucleus!

In the following comparison one can see the `ADKLinPol` ionization rates for the transition from Carbon II to III (meaning 1+ to 2+). For a reference the rates for Hydrogen as well as the barrier suppression field strengths F_{BSI} have been plotted. They mark the transition from the tunneling to the barrier suppression regime.

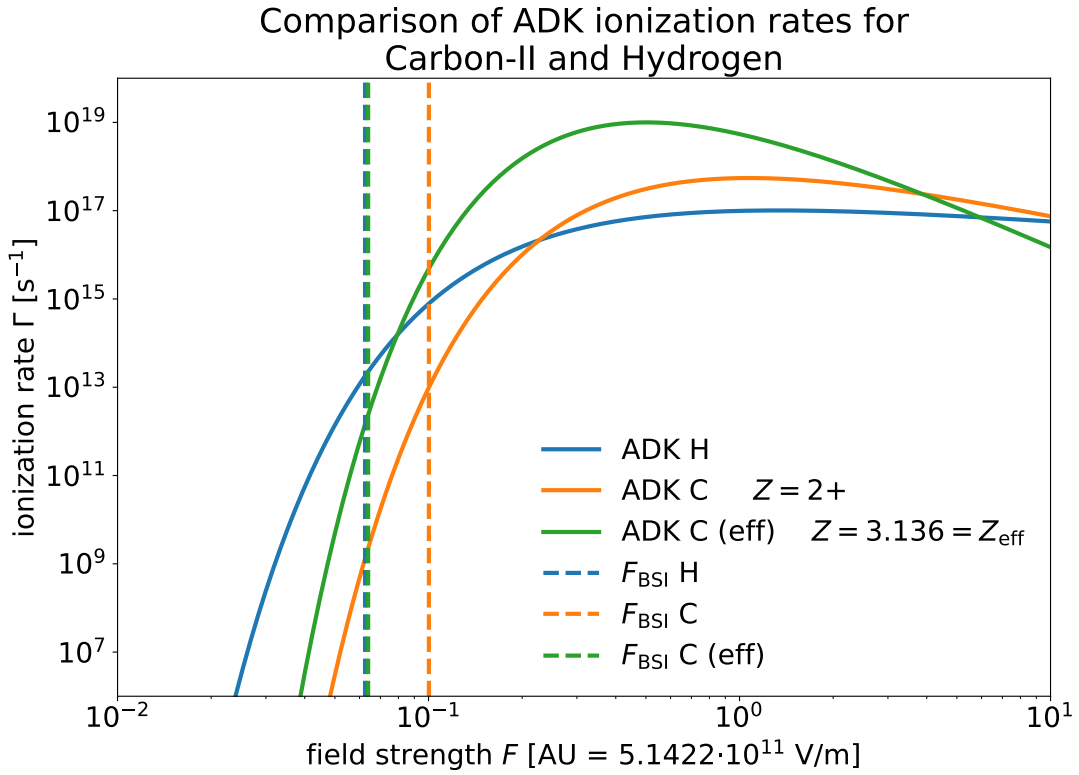
When we account for orbital structure in shielding of the ion charge Z according to [ClementiRaimondi1963] in `BSIEffectiveZ` the barrier suppression field strengths of Hydrogen and Carbon-II are very close to one another. One would expect much earlier ionization of Hydrogen due to lower ionization energy. The following image shows how this can be explained by the shape of the ion potential that is assumed in this model.

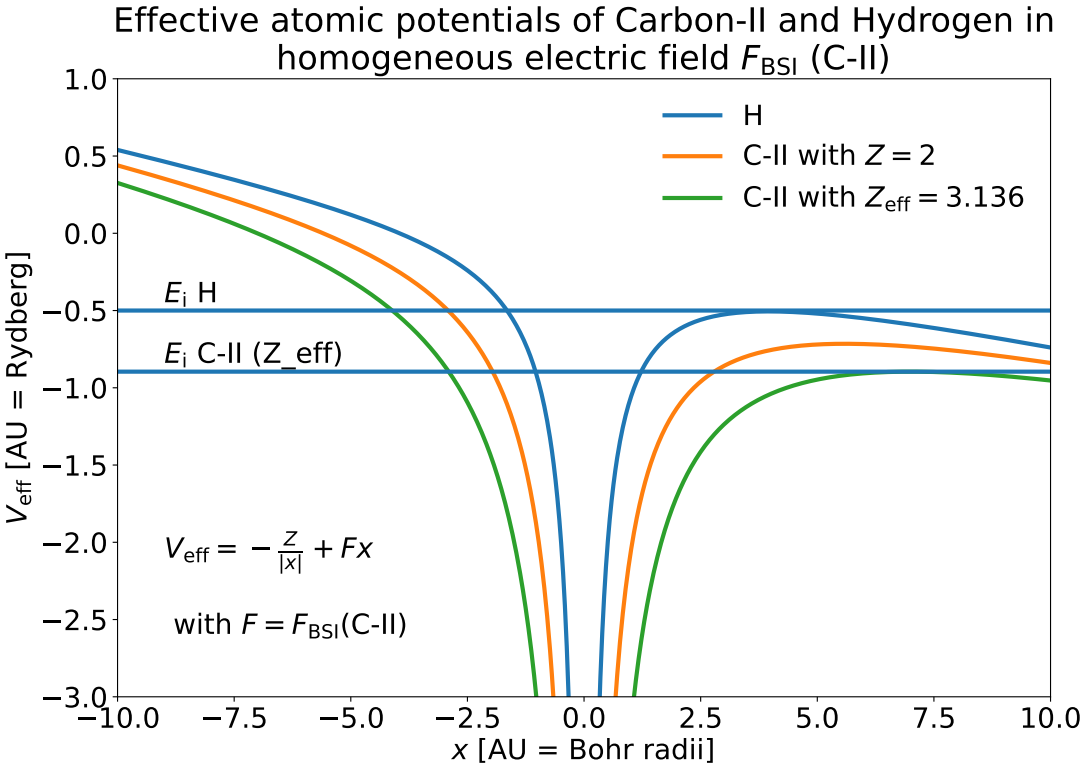
3.5.6 Predicting Charge State Distributions

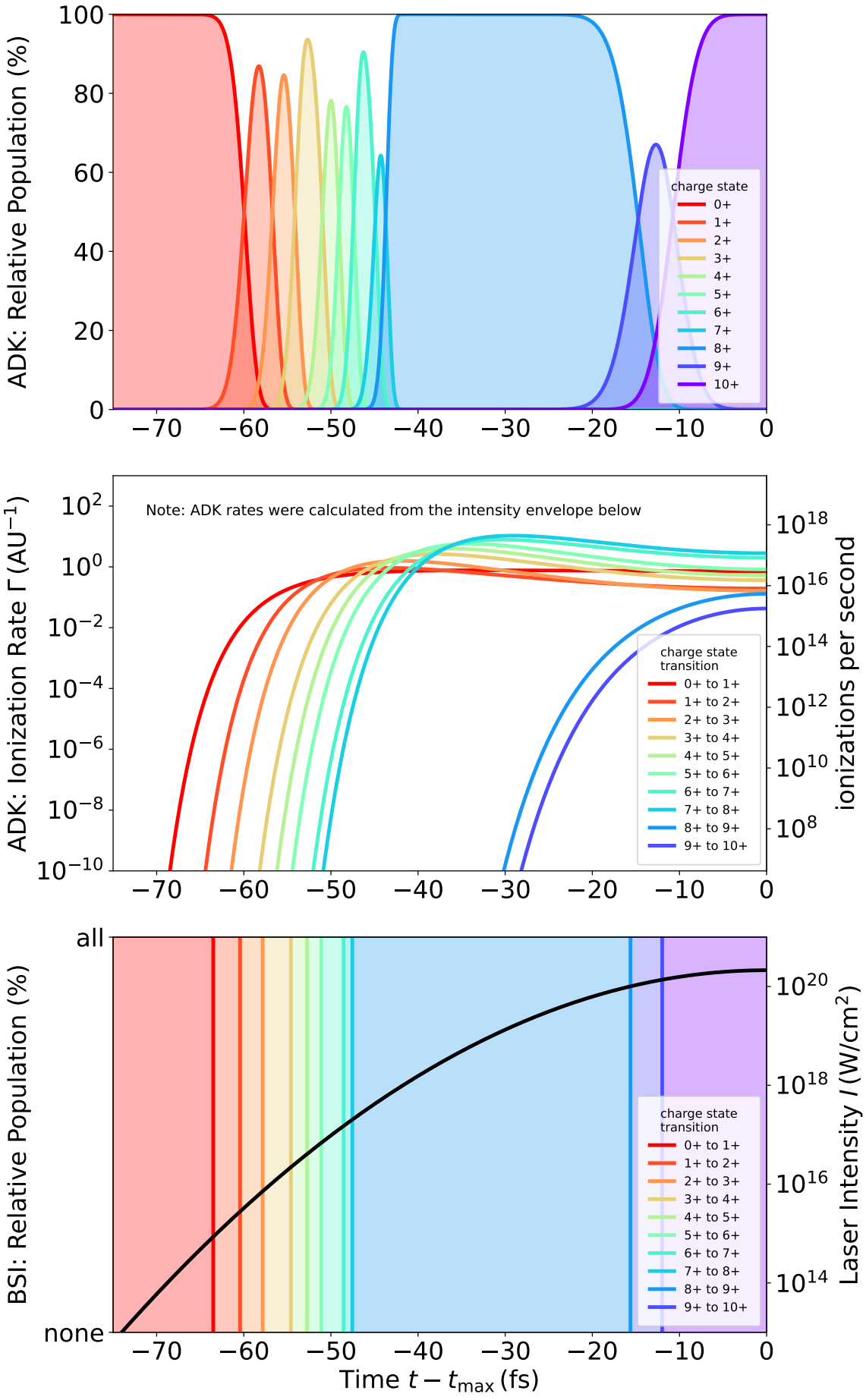
Especially for underdense targets, it is possible to already give an estimate for how the laser pulse ionizes a specific target. Starting from an initially unionized state, calculating ionization rates for each charge state for a given electric field via a Markovian approach of transition matrices yields the charge state population for each time.

Here, we show an example of Neon gas ionized by a Gaussian laser pulse with maximum amplitude $a_0 = 10$ and pulse duration (FWHM intensity) of 30 fs. The figure shows the ionization rates and charge state population produced by the `ADKLinPol` model obtained from the pulse shape in the lower panel, as well as the step-like ionization produced by the `BSI` model.

You can test the implemented ionization models yourself with the corresponding module shipped in `picongpu/lib/python`.


Comparison of ADK ionization rates for
Carbon-II and Hydrogen
ionization rate Γ [s^{-1}]
field strength F [AU = 5.1422·10^{11} V/m]
ADK H
ADK C $Z = 2+$
ADK C (eff) $Z = 3.136 = Z_{\text{eff}}$
F_{BSI} H
F_{BSI} C
F_{BSI} C (eff)


Effective atomic potentials of Carbon-II and Hydrogen in
homogeneous electric field F_{BSI} (C-II)
V_{eff} [AU = Rydberg]
x [AU = Bohr radii]
H
C-II with $Z = 2$
C-II with $Z_{\text{eff}} = 3.136$
E_{i} H
E_{i} C-II (Z_eff)
$V_{\text{eff}} = -\frac{Z}{|x|} + Fx$
with $F = F_{\text{BSI}}$(C-II)


ADK: Relative Population (%)
charge state
0+
1+
2+
3+
4+
5+
6+
7+
8+
9+
10+
Note: ADK rates were calculated from the intensity envelope below
ADK: Ionization Rate Γ (AU⁻¹)
ionizations per second
charge state transition
0+ to 1+
1+ to 2+
2+ to 3+
3+ to 4+
4+ to 5+
5+ to 6+
6+ to 7+
7+ to 8+
8+ to 9+
9+ to 10+
BSI: Relative Population (%)
all
none
Laser Intensity I (W/cm²)
Time t − t_max (fs)

```
import numpy as np
import scipy.constants as sc
from picongpu.utils import FieldIonization

# instantiate class object that contains functions for
#   - ionization rates
#   - critical field strengths (BSI models)
#   - laser intensity conversion
FI = FieldIonization()

# dictionary with atomic units
AU = FI.atomic_unit

# residual charge state AFTER ionization
Z_H = 1
# hydrogen ionization energy (13.6 eV) converted to atomic units
E_H_AU = 13.6 * sc.electron_volt / AU['energy']
# output: 0.50
print("%.2f" % (E_H_AU))
# barrier suppression threshold field strength
F_BSI_H = FI.F_crit_BSI(Z=Z_H, E_Ip=E_H_AU)
# output: 3.21e+10 V/m
print("%.2e V/m" % (F_BSI_H * AU['electric field']))
```

3.5.7 References

3.6 Collisional Ionization

3.6.1 LTE Models

Module author: Marco Garten

Implemented LTE Model: Thomas-Fermi Ionization according to [More1985]

Get started here https://github.com/ComputationalRadiationPhysics/picongpu/wiki/Ionization-in-PIConGPU

The implementation of the Thomas-Fermi model takes the following input quantities.

- ion proton number Z
- ion species mass density ρ
- electron "temperature" T

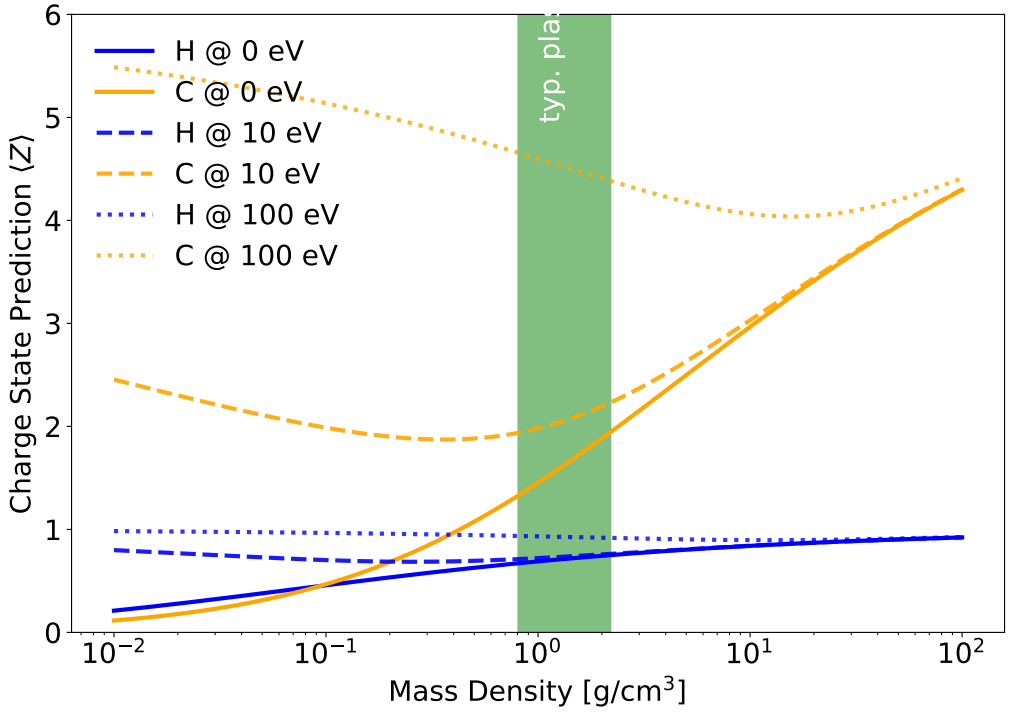
Due to the nature of our simulated setups it is also used in non-equilibrium situations. We therefore implemented additional conditions to mediate unphysical behavior but introduce arbitrariness.

Here is an example of hydrogen (in blue) and carbon (in orange) that we would use in a compound plastic target, for instance. The typical plastic density region is marked in green. Two of the artifacts can be seen in this plot:

1. Carbon is predicted to have an initial charge state $\langle Z \rangle > 0$ even at $T = 0\,\mathrm{eV}$.
2. Carbon is predicted to have a charge state of $\langle Z \rangle \approx 2$ at solid plastic density and electron temperature of $T = 10\,\mathrm{eV}$ which increases even as the density decreases. The average electron kinetic energy at such a temperature is 6.67 eV which is less than the 24.4 eV of binding energy for that state. The increase in charge state with decreasing density would lead to very high charge states in the pre-plasmas that we model.

1. Super-thermal electron cutoff

   We calculate the temperature according to $T_\mathrm{e} = \frac{2}{3} E_\mathrm{kin,e}$ in units of electron volts. We thereby assume an *ideal electron gas*. Via the variable `CUTOFF_MAX_ENERGY_KEV` in `ionizer.param` the user can exclude electrons with kinetic energy above this value from average energy



calculation. That is motivated by a lower interaction cross section of particles with high relative velocities.

2. Lower ion-density cutoff

   The Thomas-Fermi model displays unphysical behaviour for low ion densities in that it predicts an increasing charge state for decreasing ion densities. This occurs already for electron temperatures of 10 eV and the effect increases as the temperature increases. For instance in pre-plasmas of solid density targets the charge state would be overestimated where

   - on average electron energies are not large enough for collisional ionization of a respective charge state
   - ion density is not large enough for potential depression
   - electron-ion interaction cross sections are small due to small ion density

   It is strongly suggested to do approximations for **every** setup or material first. To that end, a parameter scan with [FLYCHK2005] can help in choosing a reasonable value.

3. Lower electron-temperature cutoff

   Depending on the material the Thomas-Fermi prediction for the average charge state can be unphysically high. For some materials it predicts non-zero charge states at 0 temperature. That can be a reasonable approximation for metals and their electrons in the conduction band. Yet this cannot be generalized for all materials and therefore a cutoff should be explicitly defined.

   - define via `CUTOFF_LOW_TEMPERATURE_EV` in *ionizer.param*

3.6.2 NLTE Models

Module author: Axel Huebl

in development

3.7 Photons

Section author: Axel Huebl

Module author: Heiko Burau

Radiation reaction and (hard) photons: why and when are they needed. Models we implemented ([Gonoskov] and [Furry]) and verified:

- *Landau-Lifschitz Model (semi-classical)*
- QED Models (Synchrotron & Bremsstrahlung)

Would be great to add your Diploma Thesis [Burau2016] talk with pictures and comments here.

Please add notes and warnings on the models' assumptions for an easy guiding on their usage :)

Note: Assumptions in Furry-picture and Volkov-States: classical em wave part and QED "pertubation". EM fields on grid (Synchrotron) and density modulations (Bremsstrahlung) need to be locally constant compared to radiated coherence interval ("constant-crossed-field approximation").

Attention: Bremsstrahlung: The individual electron direction and gamma emission are not correlated. (momentum is microscopically / per e- not conserved, only collectively.)

Attention: "Soft" photons from low energy electrons will get underestimated in intensity below a threshold of . . . . Their energy is still always conserved until cutoff (defined in . . .).

Note: An electron can only emit a photon with identical weighting. Otherwise, the statistical variation of their energy loss would be weighting dependent (note that the average energy loss is unaffected by that).

3.7.1 References

3.8 Binary collisions

Section author: Pawel Ordyna

Warning: This is an experimental feature. Feel free to use it but be aware that there is an unsolved bug causing some simulations to hang up. Follow the issue on github for more up to date information https://github.com/ComputationalRadiationPhysics/picongpu/issues/3461.

3.8.1 1 Introduction

The base PIC algorithm can't resolve interactions between particles, such as coulomb collisions, on a scale smaller than one cell. Taking them into consideration requires additional simulation steps. In many PIC software solutions collisions are introduced as binary collisions. With that approach every macro particle collides only with one other macro particle so that the computation time scales linearly with the number of particles, and not quadratically.

We have used the binary collisions algorithm introduced in *[1]* and updated it according to the corrections suggested in *[2]*. In that way, we were recreating the implementation from `smilei` *[3]*. We have also tested our code against `smilei` by running the test cases from `smilei`'s documentation with PIConGPU. We describe the

algorithm and the underlying equations in detail in section *3*. Section *2* explains the usage of the collision feature. We show in section *4* the test simulations that we used to compare `PIConGPU` with `smilei`.

3.8.2 2 Usage

To enable collisions in your simulation you have to edit `collision.param`. There you can define the collision initialization pipeline. The collisions are set up with the `Collider` class. Each collider defines a list of species pairs that should collide with each other. A pair can consist of two different species, for collisions between two different particle groups, or two identical species, for collision within one group. Each collider sets a fix Coulomb logarithm (automatic online estimation of the Coulomb logarithm is not yet supported). You can put in your initialization pipeline as many `Collider` objects as you need. Leaving the `CollisionPipeline` empty disables collisions.

2.1 Basics

Imagine you have two species in your simulation: `Ions` and `Electrons`. To enable collisions between the Ions and Electrons you would edit your param file in a following way:

```
namespace picongpu
{
    namespace particles
    {
        namespace collision
        {
            namespace precision
            {
                using float_COLL = float_64;
            } // namespace precision
            /** CollisionPipeline defines in which order species interact with␣
↪each other
             *
             * the functors are called in order (from first to last functor)
             */

            struct Params
            {
                static constexpr float_X coulombLog = 5.0_X;
            };
            using Pairs = MakeSeq_t<Pair<Electrons, Ions>>;
            using CollisionPipeline = bmpl::
                vector<Collider<binary::RelativisticBinaryCollision, Pairs, Params>
↪>;
        } // namespace collision
    } // namespace particles
} // namespace picongpu
```

Notice how the Coulomb logarithm is send to the collider in a struct.

If you now would like to add internal collisions (electrons – electrons and ions – ions) you just need to extend the line 20 so that it looks like that:

```
using Pairs = MakeSeq_t<Pair<Electrons, Ions>, Pair<Electrons, Electrons>, Pair
↪<Ions, Ions>>;
```

But what if you don't want to have the same Coulomb logarithm for all collision types? For that you need more colliders in your pipeline. Here is an example with $\Lambda = 5$ for electron-ion collisions and $\Lambda = 10$ for electron-electron and ion-ion collisions.

```
struct Params1
{
   static constexpr float_X coulombLog = 5.0_X;
};
struct Params2
{
   static constexpr float_X coulombLog = 10.0_X;
};
using Pairs1 = MakeSeq_t<Pair<Electrons, Ions>>;
using Pairs2 = MakeSeq_t<Pair<Electrons, Electrons>, Pair<Ions, Ions>>;
using CollisionPipeline =
    bmpl::vector<
        Collider<binary::RelativisticBinaryCollision, Pairs1, Params1>,
        Collider<binary::RelativisticBinaryCollision, Pairs2, Params2>
    >;
```

2.2 Particle filters

You can also use particle filters to further refine your setup. The `Collider` class can take one more, optional, template argument defining a pair of particle filters. Each filter is applied respectively to the first and the second species in a pair. You need to define your filters in `particleFilters.param` and than you can use them, for example, like that:

```
using Pairs1 = MakeSeq_t<Pair<Electrons, Ions>>;
using Pairs2 = MakeSeq_t<Pair<Electrons, Electrons>, Pair<Ions, Ions>>;
using CollisionPipeline =
    bmpl::vector<
        Collider<
            binary::RelativisticBinaryCollision,
            Pairs1,
            Params1,
            FilterPair<filter::FilterA, filter::FilterB>>,
        Collider<
            binary::RelativisticBinaryCollision,
            Pairs2,
            Params2,
            OneFilter<filter::FilterA>
        >;
```

Here only the electrons passing the A-filter will collide with ions but only with the ions that pass the B-filter. If the filters are identical you can use `OneFilter` instead of `FilterPair`. For collisions within one species the filters in `FilterPair` **have** to be identical since there is only one particle group colliding.

A full functional example can be found in the `CollisionsBeamRelaxation` test, where particle filters are used to enable each of the three colliders only in a certain part of the simulation box.

2.3 Precision

Highly relativistic particles can cause numerical errors in the collision algorithm that result in NaN values. To avoid that, by default, all the kinematics of a single binary collision is calculated in the 64 bit precision, regardless of the chosen simulation precision. Until now, this has been enough to avoid NaNs but we are looking into better solutions to this problem. You can change this setting by editing the

```
using float_COLL = float_64;
```

line. You can set it to

```
using float_COLL = float_X;
```

to match the simulation precision or to

```
using float_COLL = float_32;
```

for explicit single precision usage. If you use PIConGPU with the 32 bit precision, lowering the collision precision will speed up your simulation and is recommended for non–relativistic setups.

3.8.3 3 Algorithm

3.1 Algorithm overview

A short summary of the important algorithm steps in the case of inter-species collisions. The case of intra-collisions is very similar. See figures Fig. 3.1, Fig. 3.3, Fig. 3.2, Fig. 3.4 for more details.

1. Sort particles from a super cell into particle lists, one list for each grid cell.
2. In each cell, shuffle the list with more particles.
3. Collide each particle from the first longer list with a particle from the shorter one (or equally long). When you run out of particles in the shorter list, start from the beginning of that list and collide some particles more than once.
    1. Determine how many times the second particle will be collided with some particle from the longer list (in the current simulation step).
    2. Read particle momenta.
    3. Change into the center of mass frame.
    4. Calculate the s parameter.
    5. Generate a random azimuthal collision angle $\varphi \in (0, 2\pi]$.
    6. Get the cosine of the 2nd angle θ from its probability distribution (depends on s).
    7. Use the angles to calculate the final momenta (in the COM frame).
    8. Get the new momenta into the lab frame.
    9. Apply the new momentum to the macro particle A (smaller weighting).
       Do the same for the macro particle B (bigger weighting) but with a probability equal to the weighting ratio of the particles A and B.
4. Free up the memory used for the particle lists.

3.2 Details on macro particle duplication

First step that requires some more detailed explanation is the step 3.1 . In a situation where there are less macro particles, inside one cell, of one species than the other one not every macro particle has its collision partner. Similar problem emerges in a case of intra-collisions when the particle number is odd. We deal with that issue using an approach introduced in *[2]*. We collide, in such situation, some macro particles more than once. To account for that, we use corrected particle weights $w_{0/1} = \frac{1}{\max\{d_0, d_1\}}$, where $d_{0/1}$ are the number of collisions for the colliding macro particles.

Let us consider the inter-collisions first. The i–th particle from the longer list is collided with the $(i \mod m)$ –th particle in the shorter one (m is the length of the shorter list). All of the particles from the longer list will collide just once. So the correction for each binary collision is $1/d$ of the particle from the shorter list. d is determined in the following way:

```
d = floor(n / m);
if (i % m ) < (n % m) d = d + 1;
```

i – particle index in the long list, n – long list length, m – short list length, d – times the particle from the shorter list is used in the current step.

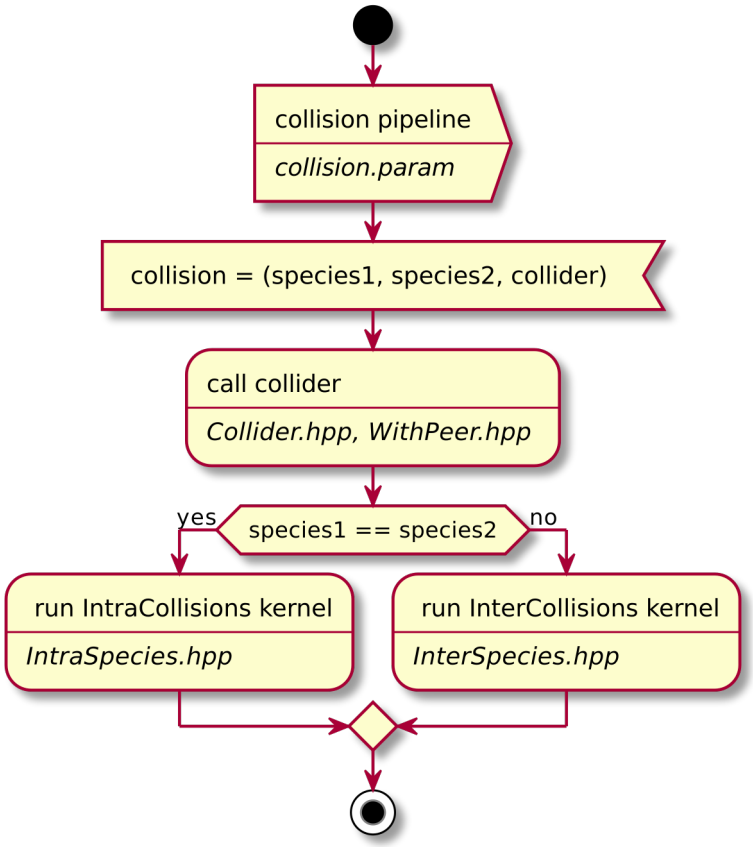


Fig. 3.1: Flow chart showing the complete algorithm. For more detail on intra-collisions see fig. Fig. 3.2, for more details on inter-collisions see fig. Fig. 3.3. Numbers in brackets refer to equations other to sections.

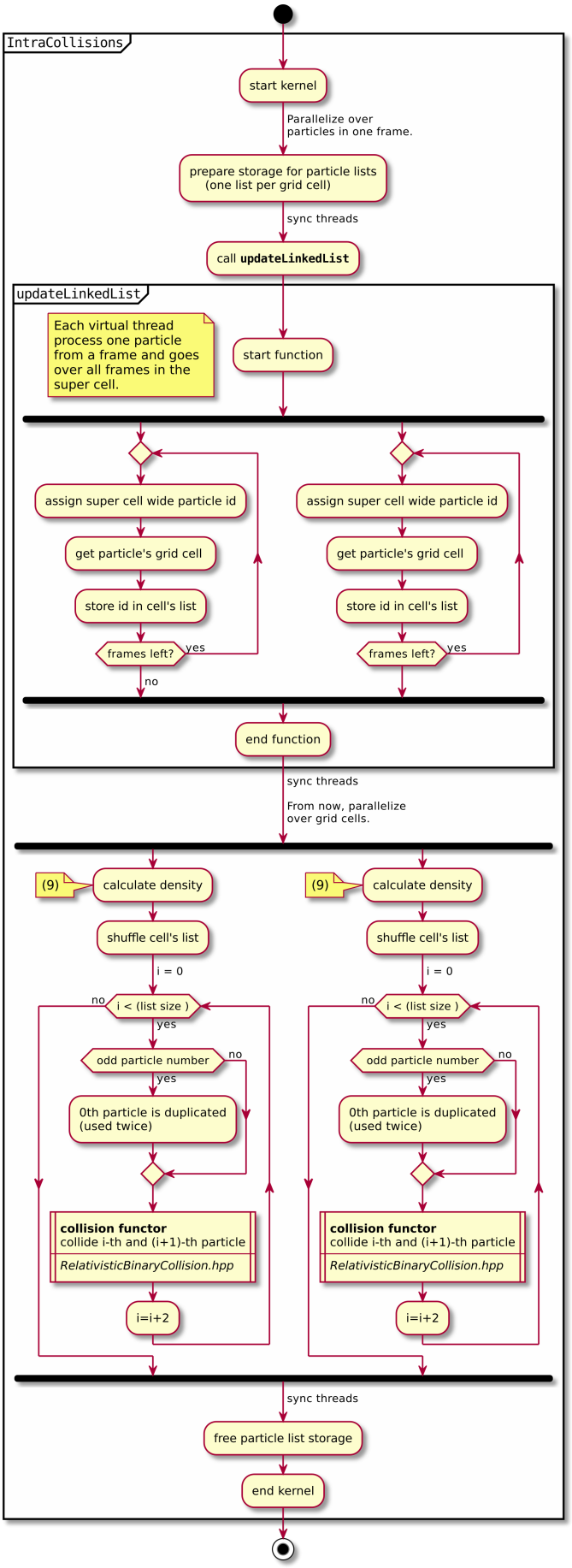


Fig. 3.2: Flow chart showing the part of the collision algorithm that is unique for intra-collisions. For more details on collisions functor see fig. Fig. 3.4 . Numbers in brackets refer to equations other to sections.

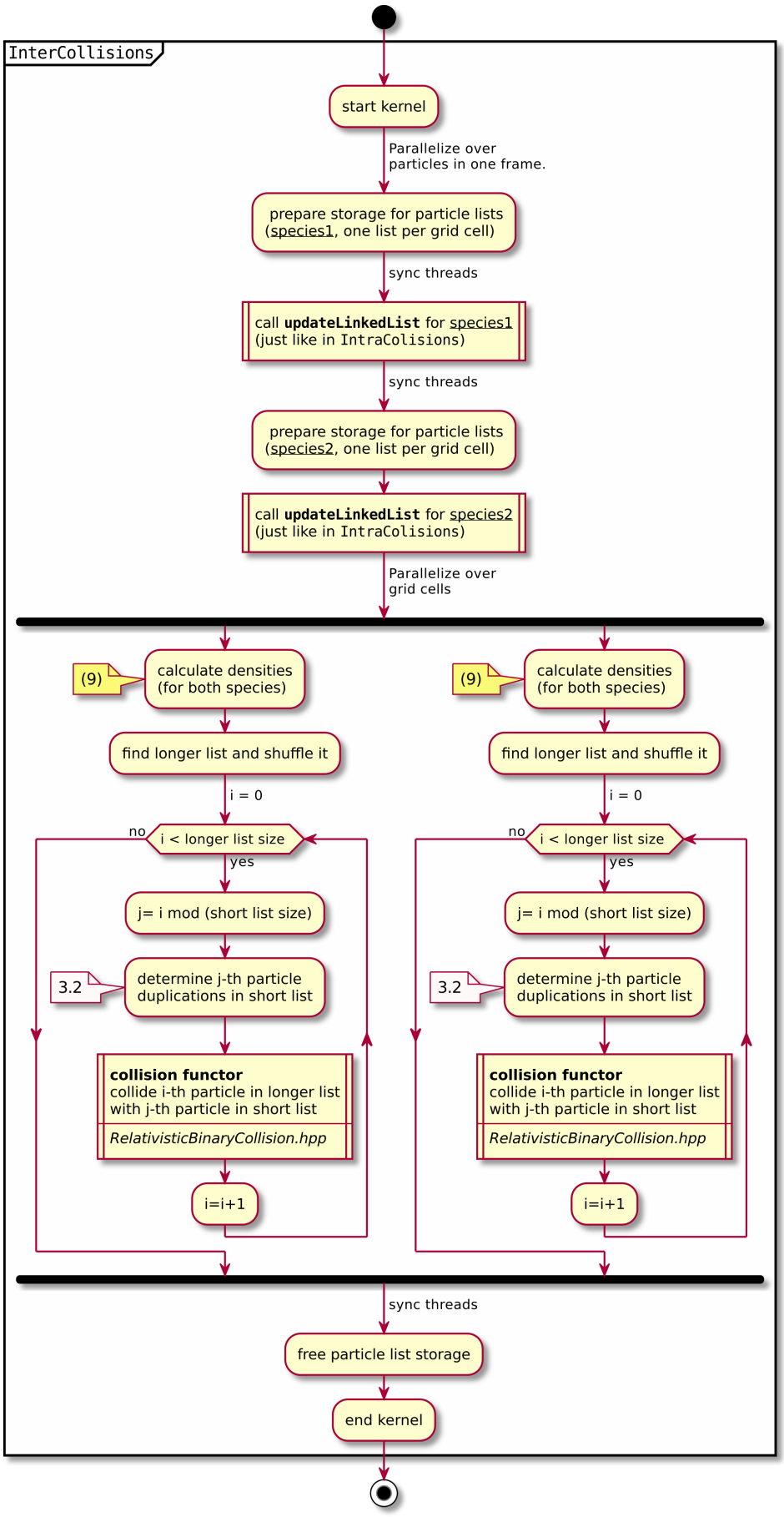


Fig. 3.3: Flow chart showing the part of the collision algorithm that is unique for inter-collisions. Numbers in brackets refer to equations other to sections.

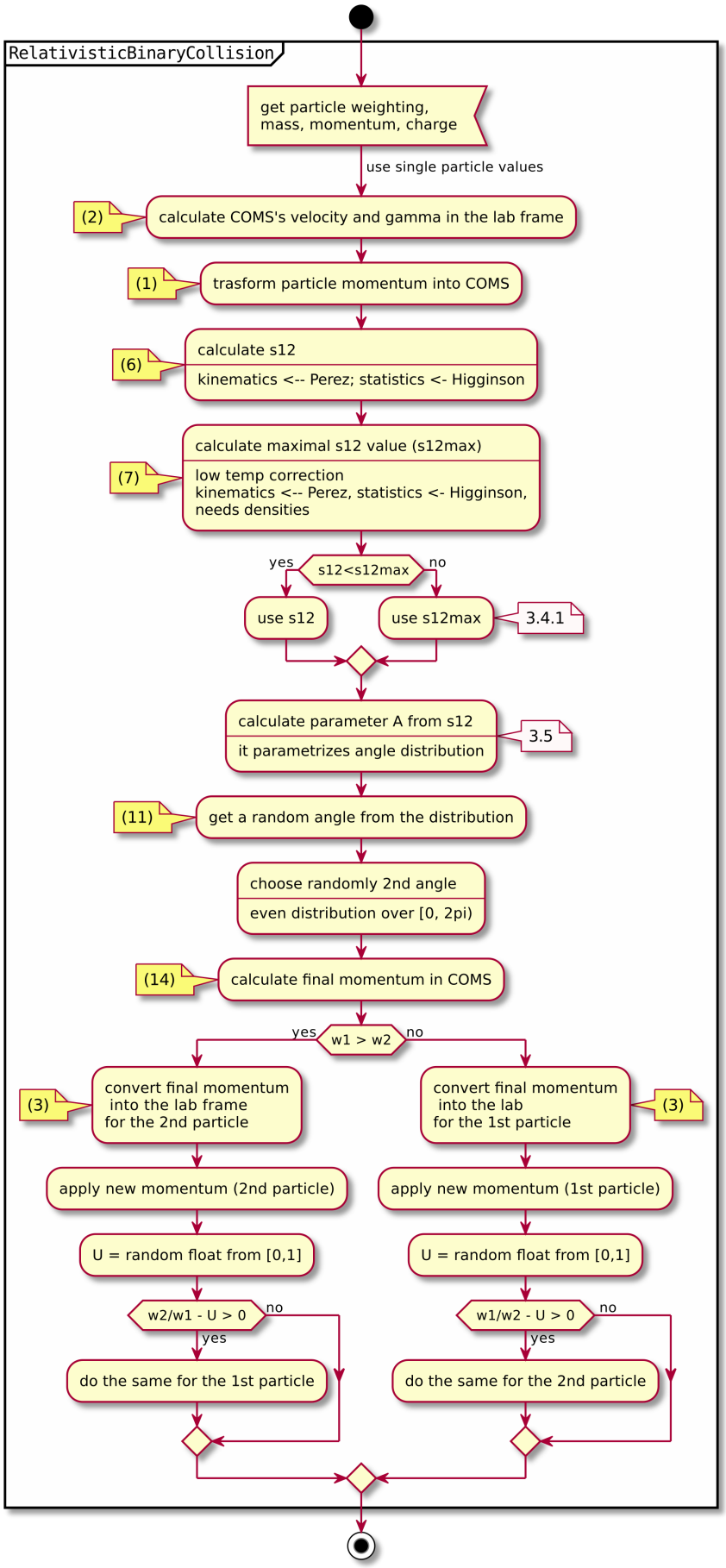


Fig. 3.4: Flow chart showing the `RelativisticBinaryCollision` collisions functor. Numbers in brackets refer to equations other to sections.

In the intra-collisions, the i–th (i is odd) particle collides with the $i+1$–th one. When there is, in total, an odd number of particles to collide, the first particle on the list collides twice. At first it is collided with the second one and in the end with the last one. All other particles collide once. So d will be 2 for the first collision (1st with 2nd particle) and for the last one (n-th with 1st particle). For the other collisions it's 1.

3.3 Details on the coordinate transform

A binary collision is calculated in this model in the center of mass frame. A star * denotes a COMS variable.

We use the coordinate transform from *[1]*:

$$\mathbf{p}^* = \mathbf{p}_{\text{lab}} + (\frac{\gamma_C - 1}{|\mathbf{v}_C|^2}\mathbf{v}_C \cdot \mathbf{v}_{\text{lab}} - \gamma_C) m\gamma\mathbf{v}_C \ , \tag{3.4}$$

where $\mathbf{v}_C$ is the velocity of the CMOS in the lab frame, γ is the [list::duplications] factor in the lab frame, m the particle mass and γ_C the gamma factor of the CMOS frame.

$$\mathbf{v}_C = \frac{\mathbf{p}_{\text{lab},0} + \mathbf{p}_{\text{lab},1}}{m_0\gamma_0 + m_1\gamma_1} \tag{3.5}$$

The inverse transformation:

$$\mathbf{p}_{\text{lab}} = \mathbf{p}^* + (\frac{\gamma_C - 1}{|\mathbf{v}_C|^2}\mathbf{v}_C \cdot \mathbf{p}^* + m\gamma^*\gamma_C)\mathbf{v}_C \ , \tag{3.6}$$

where

$$\gamma^* = \gamma_C\gamma(1 - \frac{\mathbf{v}_C \cdot \mathbf{v}_{\text{lab}}}{c^2}) \ . \tag{3.7}$$

3.4 Details on the s parameter

$$s = \frac{1}{2}N\left\langle\theta^{*2}\right\rangle \tag{3.8}$$

N is the number of real collisions. It's the number of small angle collisions of a test particle represented by one of the macro particles with all the potential collision partners in a cell (here real particles not macro particles) in the current time step assuming the relative velocity is the one of the two colliding macro particles. $\left\langle\theta^{*2}\right\rangle$ is the averaged squared scattering angle for a single collision (of real particles). According to *[2]* s is a normalized path length.

To calculate this parameter we use the relativistic formula from *[1]* and adjust it so it fits the new corrected algorithm from *[2]*.

$$\begin{aligned} s_{01} =& \frac{\Delta T \log\Lambda q_0^2 q_1^2}{4\pi\varepsilon_0^2 c^4 m_0\gamma_0 m_1\gamma_1} \\ &\times \frac{\gamma_C \left|\mathbf{p}_0^*\right|}{m_0\gamma_0 + m_1\gamma_1}(m_0\gamma_0^* m_1\gamma_1^* c^2 \left|\mathbf{p}_0^*\right|^{-2} + 1)^2 \\ &\times N_{\text{partners}} V_{\text{cell}}^{-1} \max\{\frac{w_0}{d}, \frac{w_1}{d}\} \ . \end{aligned} \tag{3.9}$$

Here: ΔT – time step duration, $\log\Lambda$ – Coulomb logarithm, q_0, q_1 – particle charges, γ_0, γ_1 particles gamma factors(lab frame), N_{partners} is the number of collision partners (macro particles), V_{cell} – cell volume, w_0, w_1 particle weightings, d was defined in 3.2.

For inter-species collisions N_{partners} is equal to the size of the long particle list. For intra-species collisions N_{partners} = $n - 1 + (n \mod 2)$,where n is the number of macro particles to collide.

The fact that s_{01} depends only on the higher weighting is accounted for by the rejection method in the 3.9 step.

3.4.1 Low temperature limit

According to *[1]* equation (3.9) will provide non physical values for low temperatures. More specifically, it will result in s values corresponding to scattering lengths smaller than the average particle distance $(\frac{V}{n})^{\frac{1}{3}}$. *[1]* provides a maximal value for s_{01}:

$$\begin{aligned} s_{01}^{\max} =& (\frac{4\pi}{3})^{1/3} \frac{\Delta T(m_0+m_1)}{\max\{m_0 n_0^{2/3}, m_1 n_1^{2/3}\}} \mathbf{v}_{\text{rel}}^* \\ & \times N_{\text{partners}} V_{\text{cell}}^{-1} \max\{\frac{w_0}{d}, \frac{w_1}{d}\} \, . \end{aligned} \tag{3.10}$$

with

$$\mathbf{v}_{\text{rel}}^* = \frac{(m_1\gamma_1 + m_2\gamma_2)p_1^*}{m_1\gamma_1^* m_2\gamma_2^* \gamma_C} \, . \tag{3.11}$$

where the relativistic factor $(1 + v_1^* v_2^*/c^2)^{-1}$ has been left out.

For each binary collision both values are calculated and the smallest one is used later. The particle density is just the sum of all particle weightings from one grid cell divided by cell volume

$$n = \frac{1}{V_{\text{cell}}} \sum_i w_i \, . \tag{3.12}$$

Note: It is not checked if the collision is really non-relativistic. If the low temp limit is smaller than s_{01} due to some other reason, e.g. an overflow in s_{01} calculation, the code will use this limit regardless of the particle being relativistic or not which could be physically incorrect.

3.5 Details on the scattering angle distribution

The distribution for the cumulative angle χ as a function of s was introduced in *[4]*

$$F(\chi) = \frac{A(s)\sin\chi}{2\sinh A(s)} e^{A(s)\cos\chi} \, . \tag{3.13}$$

We obtain a random value for the cosine from F with

$$\cos\chi = A^{-1}\ln(e^{-A} + 2U\sinh A) \, , \tag{3.14}$$

where U is a random float between 0 and 1. The parameter A is obtained by solving

$$\coth A - A^{-1} = e^{-s} \, . \tag{3.15}$$

The algorithm approximates A in a following way *[1]*

If $0.1 \leq s < 3$ then:

$$\begin{aligned} A^{-1} =& 0.0056958 + 0.9560202s \\ & - 0.508139s^2 + 0.47913906s^3 \\ & - 0.12788975s^4 + 0.02389567s^5 \, . \end{aligned} \tag{3.16}$$

If $3 \leq s < 6$ then: $A = 3e^{-s}$

For $s < 0.1$ $\cos\chi = 1 + s\ln U$ to avoid an overflow in the exponential. In the $s \to \infty$ limit scattering becomes isotropic *[4]* so that we can take $\cos\chi = 2U - 1$ for $s > 6$.

3.6 Details on final momentum calculation

The final particle momenta in the COMS frame are calculated with the following formula from *[1]*

$$\mathbf{p}_{1f}^{*} = -\mathbf{p}_{2f}^{*} = \begin{pmatrix} \frac{p_{1x}^{*} p_{1z}^{*}}{p_{1\perp}^{*}} & \frac{p_{1y}^{*} p_{1}^{*}}{p_{1\perp}^{*}} & p_{1x}^{*} \\ \frac{p_{1y}^{*} p_{1z}^{*}}{p_{1\perp}^{*}} & \frac{p_{1x}^{*} p_{1}^{*}}{p_{1\perp}^{*}} & p_{1y}^{*} \\ -p_{1\perp}^{*} & 0 & p_{1z}^{*} \end{pmatrix} \cdot \begin{pmatrix} \sin\theta^{*}\cos\varphi^{*} \\ \sin\theta^{*}\sin\varphi^{*} \\ \cos\theta^{*} \end{pmatrix} . \tag{3.17}$$

3.8.4 4 Tests

For testing we plan to reproduce all the test cases from `smilei`'s documentation(https://smileipic.github.io/Smilei/collisions.html). For now we have done the thermalization and the beam relaxation tests. The simulations that we used are available under `share/picongpu/tests`.

4.1 Thermalization

In this example there are two particle populations — electrons and ions. They are thermally initialized with different temperatures and their temperatures get closer to each other with time. The usual PIC steps are disabled (there is no field solver and no pusher). The thermalization happens solely due to the binary collisions. We enable inter-collisions for ions and electrons as well as collisions between the two species. Simulation parameters are listed in table Table 3.2. The species temperatures are calculated in post processing from an `openPMD` output. The results are shown in fig. Fig. 3.5, Fig. 3.6, and Fig. 3.7 for three different macro particle weight ratios. The theoretical curves are obtained from the same formula that was used by `smilei`'s developers and originates from the NRL plasma formulary *[5]*.

$$\frac{\mathrm{d}T_\alpha}{\mathrm{d}t} = \nu_\epsilon (T_\beta - T_\alpha)$$

$$\nu_\epsilon = \frac{2}{3}\sqrt{\frac{2}{\pi}} \frac{e^4 \, Z^{\star 2} \sqrt{m_e m_i} \, n_i \, \ln\Lambda}{4\pi\varepsilon_0^2 \, (m_e T_e + m_i T_i)^{3/2}}$$

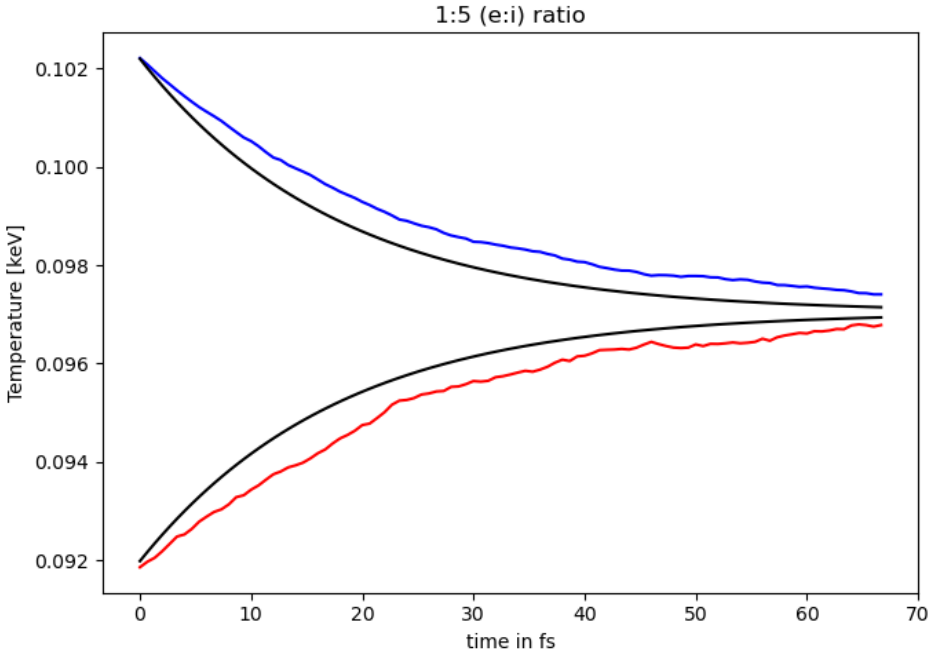


Fig. 3.5: Electron (blue) and ion (red) temperature over time in the thermalization test. The electron to ion weight ratio in the simulation is 1:5. Black lines are the the theoretical curves.

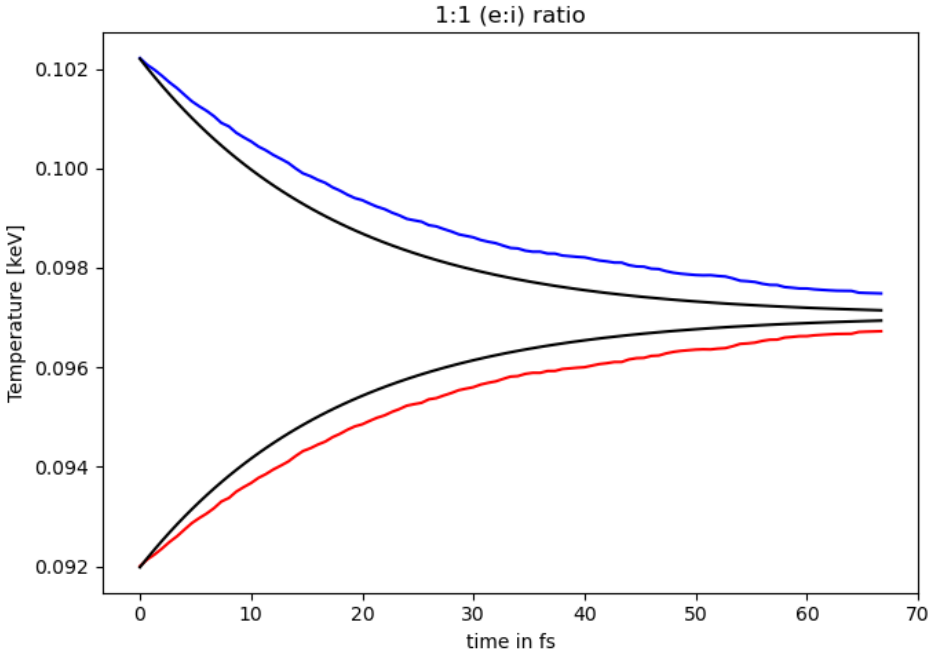


Fig. 3.6: Electron (blue) and ion (red) temperature over time in the thermalization test. The electron to ion weight ratio in the simulation is 1:1. Black lines are the the theoretical curves.

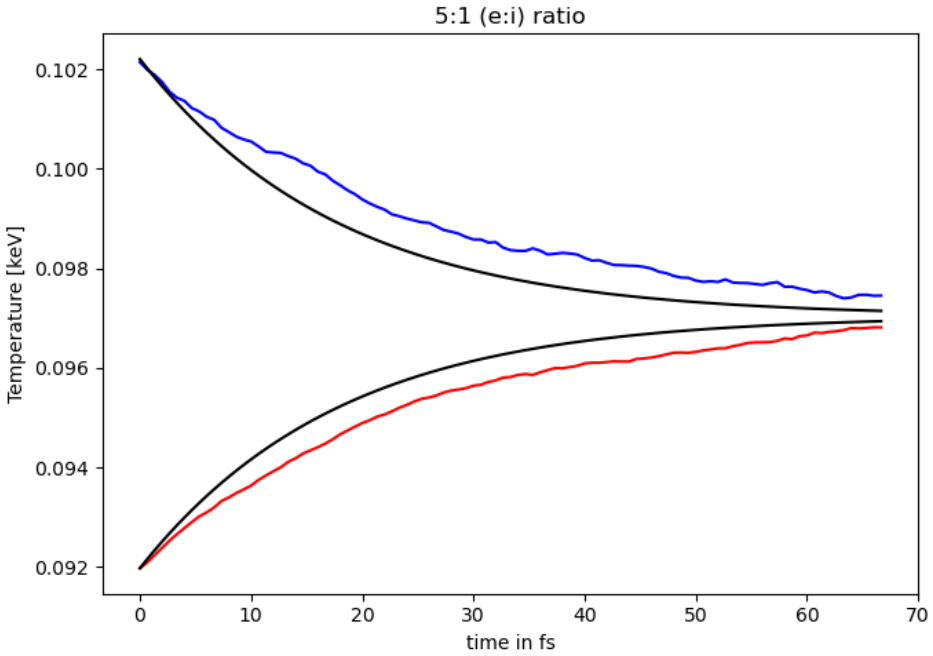


Fig. 3.7: Electron (blue) and ion (red) temperature over time in the thermalization test. The electron to ion weight ratio in the simulation is 5:1. Black lines are the the theoretical curves.

Table 3.2: Simulation parameters in the thermalization test

parameter or setting	value
time step duration	2/3 fs
time steps in the simulation	100
density profile	homogeneous
density	1.1×10^{28} m^{-3}
cell side length	$\frac{1}{3}c \cdot 10^{-13} \approx 10\mu m$
ion mass	$10\ m_e$
ion charge	+1
initial ion temperature	$1.8 \times 10^4\ m_e c^2$
initial electron temperature	$2.0 \times 10^4\ m_e c^2$
Coulomb logarithm (inter–collisions)	5
Coulomb lgarithm (intra–collisions)	1000
geometry	2D
grid	12x12
super cell size	4x4
macro particles per cell (ions) setups 1, 2, 3	5000, 1000, 5000
macro pearticles per cell (electrons) setups 1, 2, 3	5000, 5000, 1000

4.2 Beam relaxation

A population of electrons with a very small temperature and a drift velocity (the beam) is colliding with ions. Due to the collisions the velocity distribution of electrons is changing and the drift momentum is transferred into the electron transversal momentum and partially into ion momenta. In this test only the inter-collisions (between ions and electrons) are enabled.

There are three slightly different setups with varying electron drift velocity, ion charge and time step duration. Additionally each setup performs the collisions with three different electron to ion weight ratios: 1:1, 5:1, 1:5. This is achieved by dividing the simulation box into three parts and enabling collisions only for one ratio in each part. All important simulation parameters can be found in tables Table 3.3 and Table 3.4.

The figure shows the electron and ion drift velocities $\langle v_x \rangle$, electron transversal velocity $\sqrt{\langle v_\perp^2 \rangle}$, as well as the ion drift velocity, developing over time. The theoretical curves where calculated using the following formulas from the NRL formulary *[5]* :

$$\frac{\mathrm{d}v_x}{\mathrm{d}t} = \nu_s v_x$$

$$\frac{\mathrm{d}}{\mathrm{d}x}(v_{e,\perp} - \bar{v}_{e,\perp})^2 = \nu_\perp v_x^2$$

with

$$\nu_s = (1 + \frac{m_e}{m_i})\Psi(x)\nu_0$$

$$\nu_\perp = 2((1 - 0.5x)\Psi(x) + \Psi'(x))\nu_0$$

$$x = \frac{m_i v_e^2}{2k_B T_i}$$

$$v_0 = \frac{e^2 q_i^2 n_i \ln\Lambda}{4\pi\varepsilon_0 m_e^2 v_e^3}$$

$$\Psi(x) = \Gamma(\sqrt{x}) - \frac{2}{\sqrt{\pi}} e^{-x}\sqrt{x}$$

$$\Psi'(x) = \frac{2}{\sqrt{\pi}} e^{-x}\sqrt{x}\,.$$

Where v_x is the electron drift velocity and v_e is the electron drift relative to the ion background. The ion drift and ion temperature T_i are obtained from the simulation. The theory is valid only in the beginning where the velocity distribution is still more or less Maxwellian.

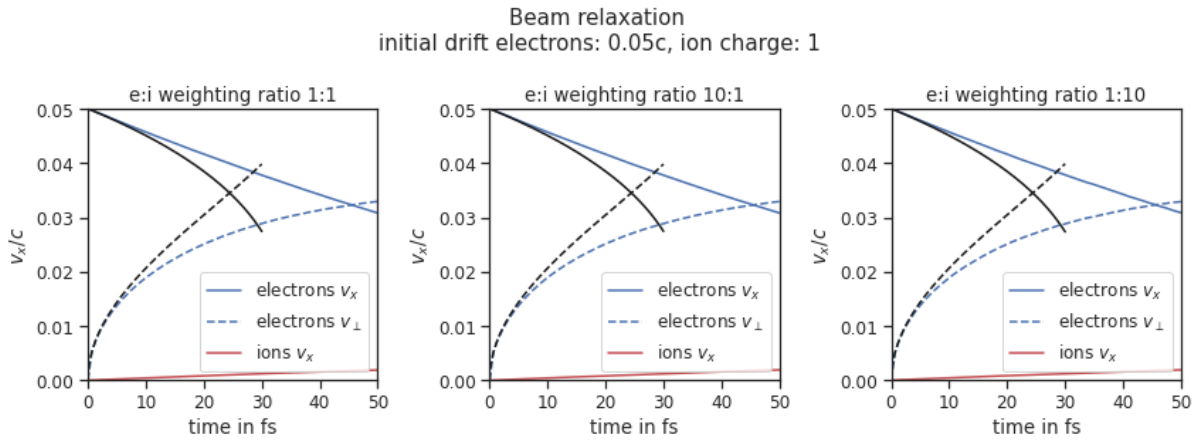


Fig. 3.8: Electron drift velocity $\langle v_x \rangle$, electron transversal velocity $\sqrt{\langle v_\perp^2 \rangle}$, and ion drift velocities from the beam equilibration example setup 1.

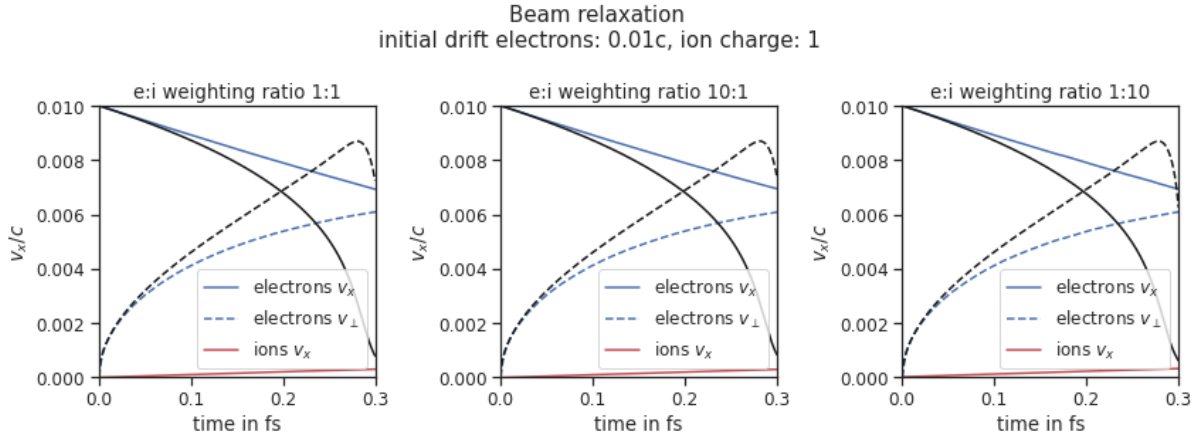


Fig. 3.9: Electron drift velocity $\langle v_x \rangle$, electron transversal velocity $\sqrt{\langle v_\perp^2 \rangle}$, and ion drift velocities from the beam equilibration example setup 2.

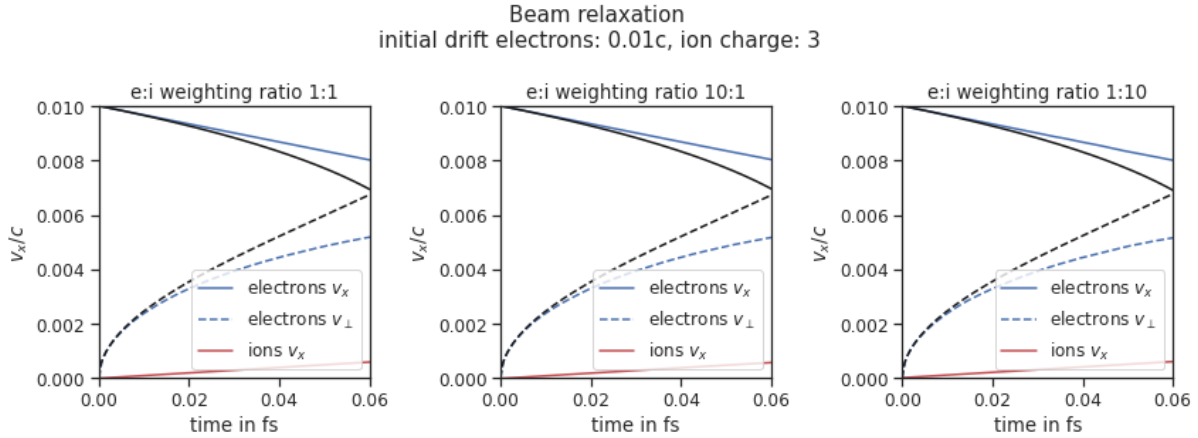


Fig. 3.10: Electron drift velocity $\langle v_x \rangle$, electron transversal velocity $\sqrt{\langle v_\perp^2 \rangle}$, and ion drift velocities from the beam equilibration example setup 3.

Table 3.3: Collisions in the 3 parts of the simulation box in the beam relaxation example

parameter	upper part	middle part	lower part
macro particles per cell (ions)	1000	1000	100
macro particles per cell (electrons)	1000	100	1000

Table 3.4: Simulation parameters in beam the relaxation test

parameter or setting	value		
	setup 1	setup 2	setup 3
time step duration	$\frac{2}{3}$ fs	$\frac{0.01}{3}$ fs	$\frac{0.002}{3}$ fs
time steps in the simulation	200		
density profile	homogeneous		
density electrons	1.1×10^{28} m^{-3}		
density ions	1.1×10^{28} m^{-3}	1.1×10^{28} m^{-3}	3.7×10^{27} m^{-3}
cell side length	$\frac{1}{15}c \cdot 10^{-13} \approx 2\mu m$		
ion mass	$10\ m_e$		
ion charge	+1	+1	+3
initial electron drift	$0.05c$	$0.01c$	$0.01c$
initial ion temperature	0.00002 $m_e c^2$		
initial electron temperature	0.0000002 $m_e c^2$		
Coulomb logarithm	5		
geometry	2D		
grid	12x12		
super cell size	4x4		

3.8.5 References

[1]F. Pérez, L. Gremillet, A. Decoster, M. Drouin, and E. Lefebvre, Improved modeling of relativistic collisions and collisional ionization in particle-in-cell codes, Physics of Plasmas 19, 083104 (2012).

[2]D. P. Higginson, I. Holod, and A. Link, A corrected method for Coulomb scattering in arbitrarily weighted particle-in-cell plasma simulations, Journal of Computational Physics 413, 109450 (2020).

[3]J. Derouillat, A. Beck, F. Pérez, T. Vinci, M. Chiaramello, A. Grassi, M. Flé, G. Bouchard, I. Plotnikov, N. Aunai, J. Dargent, C. Riconda, and M. Grech, SMILEI: A collaborative, open-source, multi-purpose particle-in-cell code for plasma simulation, Computer Physics Communications 222, 351 (2018).

[4]K. Nanbu, Theory of cumulative small-angle collisions in plasmas, Physical Review E - Statistical Physics, Plasmas, Fluids, and Related Interdisciplinary Topics 55, 4642 (1997).

[5]A. S. Richardson, NRL Plasma Formulary, (2019).

CHAPTER

FOUR

POST-PROCESSING

4.1 Python

Section author: Axel Huebl, Klaus Steiniger

If you are new to python, get your hands on the tutorials of the following important libraries to get started.

- https://www.python.org/about/gettingstarted/
- https://docs.python.org/3/tutorial/index.html

An easy way to get a Python environment for analysis of PIConGPU data up and running is to download and install Miniconda

https://docs.conda.io/en/latest/miniconda.html

and set up a conda environment with the help of this conda environment file

https://gist.github.com/steindev/d19263d41b0964bcecdfb1f47e18a86e

(see documentation within the file).

4.1.1 Numpy

Numpy is the universal swiss army knife for working on ND arrays in python.

https://docs.scipy.org/doc/numpy-dev/user/quickstart.html

4.1.2 Matplotlib

One common way to visualize plots:

- http://matplotlib.org/faq/usage_faq.html#usage
- https://gist.github.com/ax3l/fc123cb94f59d440f952

4.1.3 Jupyter

Access, share, modify, run and interact with your python scripts from your browser:

https://jupyter.readthedocs.io

4.1.4 openPMD-viewer

An exploratory framework that visualizes and analyzes data in our HDF5 files thanks to their *openPMD markup*. Automatically converts units to SI, interprets iteration steps as time series, annotates axes and provides some domain specific analysis, e.g. for LWFA. Also provides an interactive GUI for fast exploration via Jupyter notebooks.

- Project Homepage
- Tutorial

4.1.5 openPMD-api

A data library that reads (and writes) data in our openPMD files (ADIOS2 and HDF5) to and from Numpy data structures. Provides an API to correctly convert units to SI, interprets iteration steps correctly, etc.

- Manual
- Examples

4.1.6 yt-project

With yt 3.4 or newer, our HDF5 output, which uses the *openPMD markup*, can be read, processed and visualized with yt.

- Project Homepage
- Data Loading
- Data Tutorial

4.2 openPMD

Section author: Axel Huebl

Module author: Axel Huebl

If you hear about *openPMD** for the first time you can find a quick online tutorial on it here.

As a user of PIConGPU, you will be mainly interested in our *python tools* and readers, that can read openPMD, e.g. into:

- read & write data: openPMD-api (manual)
- visualization and analysis, including an exploratory Jupyter notebook GUI: openPMD-viewer (tutorial)
- yt-project (tutorial)
- *ParaView*
- VisIt
- converter tools: openPMD-converter
- full list of projects using openPMD

If you intend to write your own post-processing routines, make sure to check out our example files, the formal, open standard on openPMD and a list of projects that already support openPMD.

4.3 ParaView

Section author: Axel Huebl

Module author: Axel Huebl

Please see https://github.com/ComputationalRadiationPhysics/picongpu/wiki/ParaView for now.

CHAPTER

FIVE

USAGE FOR EXPERTS

5.1 Device Oversubscription

Module author: René Widera

By default the strategy to execute PIConGPU is that one MPI rank is using a single device e.g. a GPU. In some situation it could be beneficial to use multiple MPI ranks per device to get a better load balancing or better overlap communications with computation.

5.1.1 Usage

Follow *the description to pass command line parameter to PIConGPU*. PIConGPU provides the command line parameter `--numRanksPerDevice` or short `-r` to allow sharing a compute device between multiple MPI ranks. If you change the default value `1` to `2` PIConGPU is supporting two MPI processes per device.

Note: Using device oversubscription will limit the maximal memory footprint per PIConGPU MPI rank on the device too `<total available memory on device>/<number of ranks per device>`.

5.1.2 NVIDIA

Compute Mode

On NVIDIA GPUs there are different point which can influence the oversubscription of a device/GPU. NVIDIA Compute Mode must be `` `Default `` to allow multiple processes to use a single GPU. If you use device oversubscription with NVIDIA GPUs the kernel executed from different processes will be serialized by the driver, this is mostly describing the performance of PIConGPU because the device is under utilized.

Multi-Process Service (MPS)

If you use NVIDIA MPS and split one device into `4` you need to use `--numRanksPerDevice 4` for PIConGPU even if MPS is providing you with `4` virtual gpus. MPS can be used to workaround the kernel serialization when using multiple processes per GPU.

5.1.3 CPU

If you *compiled PIConGPU with a CPU accelerator* e.g. *omp2b*, *serial*, *tbb*, or *threads* device oversubscribing will have no effect. For CPU accelerators PIConGPU is not using a pre allocated device memory heap therefore you can freely choose the number of MPI ranks per CPU.

5.2 PIConGPU SIGNALS

Sending signals to PIConGPU allows creating checkpoints during the run and a clean shutdown before the simulation arrived the end time step. Signal support is not available on WINDOWS operating systems.

Triggering a checkpoint with signals is only possible if you enabled a *checkpointing plugin*.

5.2.1 Overview

SIGNALS handled by PIConGPU on POSIX systems

- HUP (1): Triggers USR2. Controlling process/terminal hangup.
- INT (2): Triggers USR2. This SIGNAL gets triggert while hitting ^C.
- QUIT (3): Triggers USR2. This is the terminal quit SIGNAL.
- ABRT (6): Triggers USR2. Can only be called from within the code.
- USR1 (10): Create a checkpoint for the next time step.
- USR2 (12): Finish current loop and exit normally by setting time step `n_max = n`.
- ALRM (14): Trigger USR1 and USR2.
- TERM (15): Trigger USR1.

Default SIGNALS

These can not be handled:

- KILL (9)
- CONT (18)
- STOP (19)

5.2.2 Batch Systems

Slurm

Documenation: https://slurm.schedmd.com/scancel.html

```
scancel --signal=USR1 --batch <jobid>
```

IBM LSF

Documentation: https://www.ibm.com/docs/hu/spectrum-lsf/10.1.0?topic=job-send-signal `bkill -s USR1 <jobid>`

5.2.3 Reference to SIGNALS

LINUX SIGNALS:

- https://man7.org/linux/man-pages/man7/signal.7.html
- http://en.wikipedia.org/wiki/Unix_signal#POSIX_signals

CHAPTER

SIX

DEVELOPMENT

6.1 How to Participate as a Developer

6.1.1 Contents

1. *Code - Version Control*
   - *Install git*
   - *git*
   - *git for svn users*
1. *GitHub Workflow*
   - *In a Nutshell*
   - *How to Fork From Us*
   - *Keep Track of Updates*
   - *Pull Requests or* Being Social
   - *Maintainer Notes*
1. *Commit Rules*
2. *Test Suite Examples*

6.1.2 Code - Version Control

If you are familiar with git, feel free to jump to our *github workflow* section.

install git

Debian/Ubuntu:

- `sudo apt-get install git`
- make sure `git --version` is at least at version 1.7.10

Optional *one* of these. There are nice GUI tools available to get an overview on your repository.

- `gitk git-gui qgit gitg`

Mac:

- see here

Windows:

- see here
- just kidding, it's this link
- please use ASCII for your files and take care of line endings

Configure your global git settings:

- `git config --global user.name NAME`
- `git config --global user.email EMAIL@EXAMPLE.com`
- `git config --global color.ui "auto"` (if you like colors)
- `git config --global pack.threads "0"` (improved performance for multi cores)

You may even improve your level of awesomeness by:

- `git config --global alias.pr "pull --rebase"` (see how to *avoide merge commits*)
- `git config --global alias.pm "pull --rebase mainline"` (to sync with the mainline by `git pm dev`)
- `git config --global alias.st "status -sb"` (short status version)
- `git config --global alias.l "log --oneline --graph --decorate --first-parent"` (single branch history)
- `git config --global alias.la "log --oneline --graph --decorate --all"` (full branch history)
- `git config --global rerere.enable 1` (see git rerere)
- More `alias` tricks:
  - `git config --get-regexp alias` (show all aliases)
  - `git config --global --unset alias.<Name>` (unset alias `<Name>`)

git

Git is a *distributed* **version control system**. It helps you to keep your software development work organized, because it keeps track of *changes* in your project. It also helps to come along in **teams**, crunching on the *same project*. Examples:

- Arrr, dare you other guys! Why did you change my precious *main.cpp*, too!?
- Who introduced that awesome block of code? I would like to pay for a beer as a reward.
- Everything is wrong now, why did this happen and when?
- What parts of the code changed since I went on vacation (to a conference, phd seminar, mate fridge, . . .)?

If *version control* is totally **new** to you (that's good, because you are not spoiled) - please refer to a beginners guide first.

- git - the simple guide
- 15 minutes guide at try.github.io

Since git is *distributed*, no one really needs a server or services like github.com to *use git*. Actually, there are even very good reasons why one should use git even for **local** data, e.g. a master thesis (or your collection of ascii art dwarf hamster pictures).

Btw, **fun fact warning**: Linus Torvalds, yes the nice guy with the pinguin stuff and all that, developed git to maintain the **Linux kernel**. So that's cool, by definition.

A nice overview about the *humongous* number of tutorials can be found at stackoverflow.com . . . but we may like to start with a git **cheat sheet** (is there anyone out there who knows more than 1% of all git commands available?)

- git-tower.com (print the 1st page)

- github.com - "cheat git" gem (a cheat sheet for the console)
- kernel.org *Everyday GIT with 20 commands or so*
- an other interactive, huge cheat sheet (nice overview about stash - workspace - index - local/remote repositories)

Please spend a minute to learn how to write **useful** git commit **messages** (caption-style, maximum characters per line, use blank lines, present tense). Read our *commit rules* and use keywords.

If you like, you can **credit** someone else for your **next commit** with:

- `git commit --author "John Doe <johns-github-mail@example.com>"`

git for svn users

If you already used version control systems before, you may enjoy the git for svn users crash course.

Anyway, please keep in mind to use git *not* like a centralized version control system (e.g. *not* like svn). Imagine git as your *own private* svn server waiting for your commits. For example *Github.com* is only **one out of many** *sources for updates*. (But of course, we agree to share our *finished*, new features there.)

6.1.3 GitHub Workflow

Welcome to github! We will try to explain our coordination strategy (I am out of here!) and our development workflow in this section.

In a Nutshell

Create a *GitHub* account and prepare your *basic git config*.

Prepare your *forked* copy of our repository:

- fork picongpu on *GitHub*
- `git clone git@github.com:<YourUserName>/picongpu.git` (create local copy)
- `git remote add mainline git@github.com:ComputationalRadiationPhysics/picongpu.git` (add our main repository for updates)
- `git checkout dev` (switch to our, its now *your*, dev branch to start from)

Start a *topic/feature branch*:

- `git checkout -b <newFeatureName>` (start a new branch from dev and check it out)
- *hack hack*
- `git add <yourChangedFiles>` (add changed and new files to index)
- `git clang-format` (format all changed files with the clang-format utility, needs to be loaded or installed separately)
- `git add <yourChangedFiles>` (add the formating changes)
- `git commit` (commit your changes to your *local* repository)
- `git pull --rebase mainline dev` (update with our *remote dev* updates and avoid a merge commit)

Optional, *clean up* your feature branch. That can be *dangerous*:

- `git pull` (if you pushed your branch already to your public repository)
- `git pull --rebase mainline dev` (apply the mainline updates to your feature branch)

- `git log ..mainline/dev`, `git log --oneline --graph --decorate --all` (check for related commits and ugly merge commits)
- `git rebase mainline/dev` (re-apply your changes after a fresh update to the `mainline/dev`, see here)
- `git rebase -i mainline/dev` (squash related commits to reduce the complexity of the features history during a pull request)

Publish your feature and start a *pull request*:

- `git push -u origin <newFeatureName>` (push your local branch to your github profile)
- Go to your *GitHub* page and open a *pull request*, e.g. by clicking on *compare & review*
- Select `ComputationalRadiationPhysics:dev` instead of the default `master` branch
- Add additional updates (if requested to do so) by `push`-ing to your branch again. This will update the *pull request*.

How to fork from us

To keep our development fast and conflict free, we recomment you to fork our repository and start your work from our **dev** (development) branch in your private repository. Simply click the *Fork* button above to do so.

Afterwards, `git clone` **your** repository to your local machine. But that is not it! To keep track of the original **dev** repository, add it as another remote.

- `git remote add mainline https://github.com/ComputationalRadiationPhysics/picongpu.git`
- `git checkout dev` (go to branch **dev**)

Well done so far! Just start developing. Just like this? No! As always in git, start a *new branch* with `git checkout -b topic-<yourFeatureName>` and apply your changes there.

Keep track of updates

We consider it a **best practice** *not to modify* neither your **master** nor your **dev** branch at all. Instead you can use it to `pull --ff-only` new updates from the original repository. Take care to **switch to dev** by `git checkout dev` to start **new feature branches** from **dev**.

So, if you like to do so, you can even keep track of the *original dev* branch that way. Just start your new branch with `git branch --track <yourFeatureName> mainline/dev` instead. This allows you to immediatly pull or fetch from **our dev** and avoids typing (during `git pull --rebase`). Nevertheless, if you like to `push` to *your* forked (== `origin`) repository, you have to say e.g. `git push origin <branchName>` explicitly.

You should **add updates** from the original repository on a **regular basis** or *at least* when you *finished your feature*.

- commit your local changes in your *feature branch*: `git commit`

Now you *could* do a normal *merge* of the latest `mainline/dev` changes into your feature branch. That is indeed possible, but will create an ugly merge commit. Instead try to first update *the point where you branched from* and apply your changes *again*. That is called a **rebase** and is indeed less harmful as reading the sentence before:

- `git checkout <yourFeatureName>`
- `git pull --rebase mainline dev` (in case of an emergency, hit `git rebase --abort`)

Now solve your conflicts, if there are any, and you got it! Well done!

Pull requests or *being social*

How to propose that **your awesome feature** (we know it will be awesome!) should be included in the **mainline PIConGPU** version?

Due to the so called pull requests in *GitHub*, this quite easy (yeah, sure). We start again with a *forked repository* of our own. You already created a **new feature branch** starting from our **dev** branch and commited your changes. Finally, you publish you local branch via a *push* to *your* GitHub repository: `git push -u origin <yourLocalBranchName>`

Now let's start a *review*. Open the *GitHub* homepage, go to your repository and switch to your *pushed feature branch*. Select the green **compare & review** button. Now compare the changes between **your feature branch** and **our dev**.

Everything looks good? Submit it as a **pull request** (link in the header). Please take the time to write an **extensive description**.

- What did you implement and why?
- Is there an open issue that you try to address (please link it)?
- Do not be afraid to add images!

The description of the pull request is essential and will be referred to in the change log of the next release.

Please consider to change only **one aspect per pull request** (do not be afraid of follow-up pull requests!). For example, submit a pull request with a bug fix, another one with new math implementations and the last one with a new awesome implementation that needs both of them. You will see, that speeds up *review time* a lot!

Speaking of those, a fruitful (*wuhu, we love you - don't be scared*) *discussion* about your **submitted change set** will start at this point. If we find some things you could *improve* (*That looks awesome, all right!*), simply change your *local feature branch* and *push the changes back* to your GitHub repository, to **update the pull request**. (You can now rebase follow-up branches, too.)

One of our maintainers will pick up the pull request to coordinate the review. Other regular developers that are competent in the topic might assist.

Sharing is caring! Thank you for participating, **you are great**!

maintainer notes

- do not *push* to the main repository on a regular basis, use **pull request** for your features like everyone else
- **never** do a *rebase* on the mainline repositories (this causes heavy problems for everyone who pulls them)
- on the other hand try to use pull –rebase to **avoid merge commits** (in your *local/topic branches* **only**)
- do not vote on your *own pull requests*, wait for the other maintainers
- we try to follow the strategy of a-successful-git-branching-model

Last but not least, help.github.com has a very nice FAQ section.

More best practices.

6.1.4 Commit Rules

See our commit rules page

6.1.5 Test Suite Examples

You know a useful setting to validate our provided methods? Tell us about it or add it to our test sets in the examples/ folder!

6.2 PIConGPU Commit Rulez

We agree on the following simple rules to make our lives easier :)

- Stick to the **style** below for **commit messages**
- **Commit compiling patches** for the *main* branches (`master` and `dev`), you can be less strict for (unshared) *topic branches*
- Commits should be formated with clang-format-11

6.2.1 Format Code

- Install *ClangFormat 11*
- To format all files in your working copy, you can run this command in bash from the root folder of PIConGPU:

```
find include/ share/picongpu/ share/pmacc -iname "*.def" \
-o -iname "*.h" -o -iname "*.cpp" -o -iname "*.cu" \
-o -iname "*.hpp" -o -iname "*.tpp" -o -iname "*.kernel" \
-o -iname "*.loader" -o -iname "*.param" -o -iname "*.unitless" \
| xargs clang-format-11 -i
```

Instead of using the bash command above you can use *Git* together with *ClangFormat* to format your patched code only. Before applying this command, you must extend your local git configuration **once** with all file endings used in *PIConGPU*:

```
git config --local clangFormat.extensions def,h,cpp,cu,hpp,tpp,kernel,loader,param,
↪unitless
```

For only formatting lines you added using `git add`, call `git clang-format-11` before you create a commit. Please be aware that un-staged changes will not be formatted.

6.2.2 Commit Messages

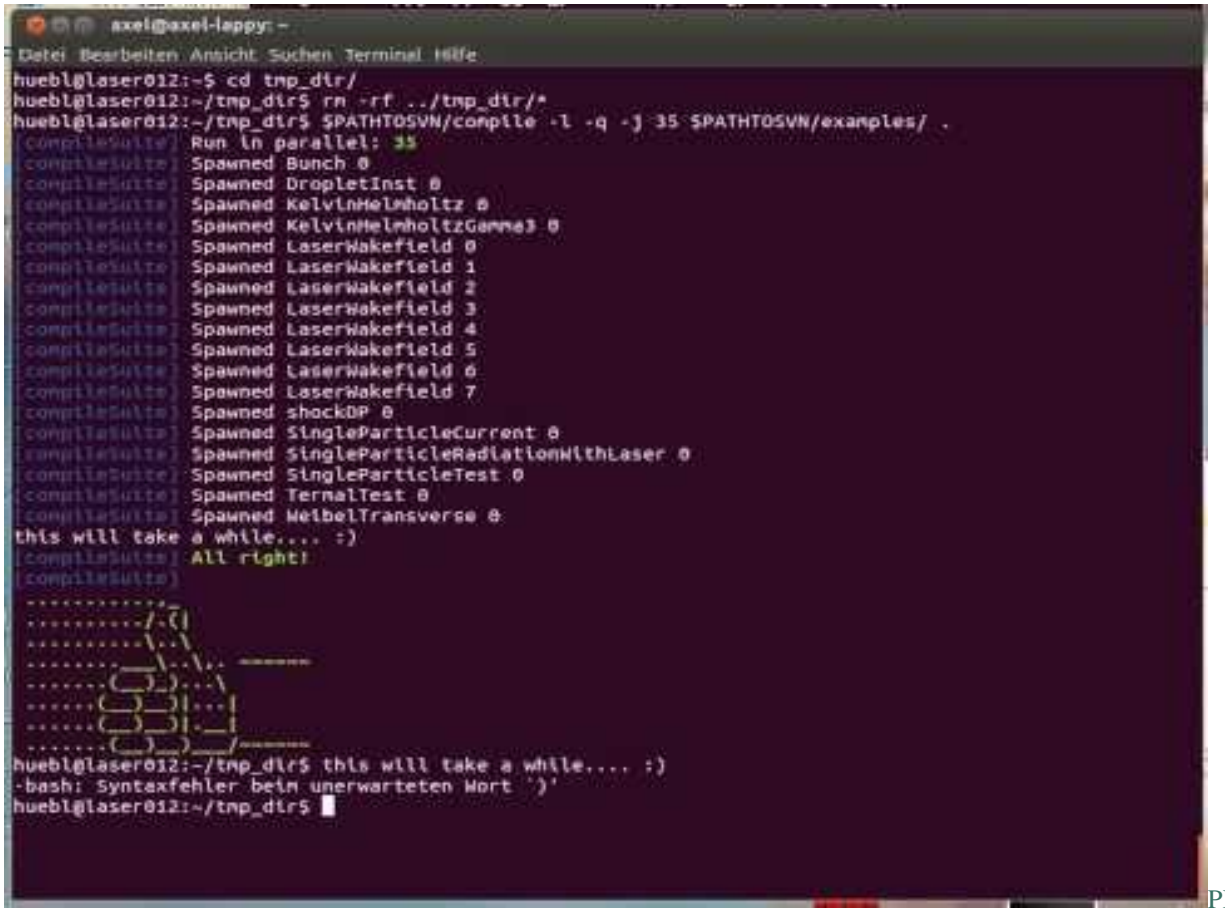
Let's go for an example:

> Use the 1st line as a topic, stay <= 50 chars
>
> - the blank line between the "topic" and this "body" is MANDATORY
> - use several key points with - or * for additional information
> - stay <= 72 characters in this "body" section
> - avoid blank lines in the body
> - Why? Pls refer to http://stopwritingramblingcommitmessages.com/

6.2.3 Compile Tests

We provide an (interactive/automated) **script** that **compiles all examples** within the `examples/` directory in your branch.

This helps a lot to **maintain various combinations** of options in the code (like different solvers, boundary conditions, . . .).



PIConGPU CompileTest

Assume

- `repo=<pathToYourPIConGPUgitDirectory>`
- `tmpPath=<tmpFolder>`

Now run the tests with

- `$repo/compile -l $repo/examples/ $tmpPath`

Further options are:

- `-q :  continue on errors`
- `-j <N> :  run <N> tests in parallel (note:  do NOT omit the number <N>)`

If you ran your test with, let's say `-l -q -j 4`, and you got errors like

> [compileSuite] [error] In PIC_EXTENSION_PATH:PATH=. . . /params/ThermalTest/cmakePreset_0: CMAKE_INSTALL_PREFIX:PATH=. . . /params/ThermalTest/cmakePreset_0 (. . . /build) make install

check the specific test's output (in this case `examples/ThermalTest` with *CMake preset #0*) with:

- `less -R $tmpPath/build/build_ThermalTest_cmakePreset_0/compile.log`

Compile Tests - Single Example

Compile **all CMake presets** of a *single example* with:

- `$repo/compile $repo/examples/ $tmpPath`

Compile Tests - Cluster Example:

- Request an interactive job (to release some load from the head node) `qsub -I -q laser -lwalltime=03:00:00 -lnodes=1:ppn=64`
- Use a non-home directory, e.g. `tmpPath=/net/cns/projects/HPL/<yourTeam>/<yourName>/tmp_tests/`
- Compile like a boss! `<pathToYourPIConGPUgitDirectory>/compile -l -q -j 60 <pathToYourPIConGPUgitDirectory>/examples/ $tmpPath`
- Wait for the **thumbs up/down** :)

6.3 Repository Structure

Section author: Axel Huebl

6.3.1 Branches

- `master`: the latest stable release, always tagged with a version
- `dev`: the development branch where all features start from and are merged to
- `release-X.Y.Z`: release candiate for version `X.Y.Z` with an upcoming release, receives updates for bug fixes and documentation such as change logs but usually no new features

6.3.2 Directory Structure

- `include/`
  - C++ header *and* source files
  - set `-I` here
  - prefixed with project name
- `lib/`
  - pre-compiled libraries
  - `python/`
    - modules, e.g. for RT interfaces, pre* & post-processing
    - set `PYTHONPATH` here
- `etc/`
  - (runtime) configuration files
  - `picongpu/`
    - `tbg` templates (as long as PIConGPU specific, later on to `share/tbg/`)
    - network configurations (e.g. infiniband)
    - score-p and vampir-trace filters
- `share/`
  - examples, documentation
  - `picongpu/`
    - `completions/`: bash completions
    - `examples/`: each with same structure as `/`

- `bin/`
  - core tools for the "PIConGPU framework"
  - set `PATH` here
- `docs/`
  - currently for the documentation files
  - might move, e.g. to `lib/picongpu/docs/` and its build artifacts to `share/{doc,man}/`,

6.4 Coding Guide Lines

Section author: Axel Huebl

See also:

Our coding guide lines are documented in this repository.

6.4.1 Source Style

For contributions, *an ideal patch blends in the existing coding style around it* without being noticed as an addition when applied. Nevertheless, please make sure *new files* follow the styles linked above as strict as possible from the beginning.

clang-format-11 should be used to format the code. There are different ways to format the code.

Format All Files

To format all files in your working copy, you can run this command in bash from the root folder of PIConGPU:

```
find include/ share/picongpu/ share/pmacc -iname "*.def" \
  -o -iname "*.h" -o -iname "*.cpp" -o -iname "*.cu" \
  -o -iname "*.hpp" -o -iname "*.tpp" -o -iname "*.kernel" \
  -o -iname "*.loader" -o -iname "*.param" -o -iname "*.unitless" \
  | xargs clang-format-11 -i
```

Format Only Changes, Using Git

Instead of using the bash command above you can use *Git* together with *ClangFormat* to format your patched code only.

> *ClangFormat* is an external tool for code formating that can be called by *Git* on changed files only and is part of clang tools.

Before applying this command, you must extend your local git configuration **once** with all file endings used in *PIConGPU*:

```
git config --local clangFormat.extensions def,h,cpp,cu,hpp,tpp,kernel,loader,param,
↪unitless
```

After installing, or on a cluster loading the module(see introduction), clangFormat can be called by git on all **staged files** using the command:

```
git clangFormat
```

Warning: The binary for *ClangFormat* is called *clang-format* on some operating systems. If *clangFormat* is not recognized, try *clang-format* instead, in addition please check that *clang-format –version* returns version *11.X.X* in this case.

The Typical workflow using git clangFormat is the following,

1. make your patch
2. stage the changed files in git

```
git add <files you changed>/ -A
```

3. format them according to guidelines

```
git clangFormat
```

4. stage the now changed(formated) files again

```
git add <files you changed>
```

5. commit changed files

```
git commit -m <commit message>
```

Please be aware that un-staged changes will not be formatted. Formatting all changes of the previous commit can be achieved by executing the command *git clang-format-11 HEAD~1*.

6.4.2 License Header

Please **add the according license header** snippet to your *new files*:

- for PIConGPU (GPLv3+): `src/tools/bin/addLicense <FileName>`
- for libraries (LGPLv3+ & GPLv3+): `export PROJECT_NAME=PMacc && src/tools/bin/addLicense <FileName>`
- delete other headers: `src/tools/bin/deleteHeadComment <FileName>`
- add license to all `.hpp` files within a directory (recursive): `export PROJECT_NAME=PIConGPU && src/tools/bin/findAndDo <PATH> "*.hpp" src/tools/bin/addLicense`
- the default project name is `PIConGPU` (case sensitive!) and add the GPLv3+ only

Files in the directory `thirdParty/` are only imported from remote repositories. If you want to improve them, submit your pull requests there and open an issue for our **maintainers** to update to a new version of the according software.

6.5 Sphinx

Section author: Axel Huebl, Marco Garten

In the following section we explain how to contribute to this documentation.

If you are reading the HTML version on http://picongpu.readthedocs.io and want to improve or correct existing pages, check the "Edit on GitHub" link on the right upper corner of each document.

Alternatively, go to *docs/source* in our source code and follow the directory structure of reStructuredText (`.rst`) files there. For intrusive changes, like structural changes to chapters, please open an issue to discuss them beforehand.

6.5.1 Build Locally

This document is build based on free open-source software, namely Sphinx, Doxygen (C++ APIs as XML) and Breathe (to include doxygen XML in Sphinx). A web-version is hosted on ReadTheDocs.

The following requirements need to be installed (once) to build our documentation successfully:

```
cd docs/

# doxygen is not shipped via pip, install it externally,
# from the homepage, your package manager, conda, etc.
# example:
sudo apt-get install doxygen

# python tools & style theme
pip install -r requirements.txt # --user
```

In order to not break any of your existing Python configurations, you can also create a new environment that you only use for building the documentation. Since it is possible to install doxygen with conda, the following demonstrates this.

```
cd docs/

# create a bare conda environment containing just all the requirements
# for building the picongpu documentation
# note: also installs doxygen inside this environment
conda env create --file picongpu-docs-env.yml

# start up the environment as suggested during its creation e.g.
conda activate picongpu-docs-env
# or
source activate picongpu-docs-env
```

With all documentation-related software successfully installed, just run the following commands to build your docs locally. Please check your documentation build is successful and renders as you expected before opening a pull request!

```
# skip this if you are still in docs/
cd docs/

# parse the C++ API documentation,
#   enjoy the doxygen warnings!
doxygen
# render the `.rst` files and replace their macros within
#   enjoy the breathe errors on things it does not understand from doxygen :)
make html

# open it, e.g. with firefox :)
firefox build/html/index.html

# now again for the pdf :)
make latexpdf

# open it, e.g. with okular
build/latex/PIConGPU.pdf
```

6.5.2 Useful Links

- A primer on writing restFUL files for sphinx
- Why You Shouldn't Use "Markdown" for Documentation

- Markdown Limitations in Sphinx

6.6 Doxygen

Section author: Axel Huebl

An online version of our Doxygen build can be found at

http://computationalradiationphysics.github.io/picongpu

We regularly update it via

```
git checkout gh-pages

# optional argument: branch or tag name
./update.sh

git commit -a
git push
```

This section explains what is done when this script is run to build it manually.

6.6.1 Requirements

First, install Doxygen and its dependencies for graph generation.

```
# install requirements (Debian/Ubuntu)
sudo apt-get install doxygen graphviz

# enable HTML output in our Doxyfile
sed -i 's/GENERATE_HTML.*=.*NO/GENERATE_HTML     = YES/' docs/Doxyfile
```

6.6.2 Build

Now run the following commands to build the Doxygen HTML documentation locally.

```
cd docs/

# build the doxygen HTML documentation
doxygen

# open the generated HTML pages, e.g. with firefox
firefox html/index.html
```

6.7 Clang Tools

Section author: Axel Huebl

We are currently integrating support for Clang Tools [ClangTools] such as `clang-tidy` and `clang-format`. Clang Tools are fantastic for static source code analysis, e.g. to find defects, automate style formatting or modernize code.

6.7.1 Install

At least LLVM/Clang 3.9 or newer is required. On Debian/Ubuntu, install them via:

```
sudo apt-get install clang-tidy-3.9
```

6.7.2 Usage

Currently, those tools work only with CPU backends of PIConGPU. For example, enable the *OpenMP* backend via:

```
# in an example
mkdir .build
cd build

pic-configure -c"-DALPAKA_ACC_CPU_B_OMP2_T_SEQ_ENABLE=ON" ..
```

We try to auto-detect `clang-tidy`. If that fails, you can set a manual hint to an adequate version via `-DCLANG_TIDY_BIN` in CMake:

```
pic-configure -c"-DALPAKA_ACC_CPU_B_OMP2_T_SEQ_ENABLE=ON -DCLANG_TIDY_BIN=$(which␣
↪clang-tidy-3.9)" ..
```

If a proper version of `clang-tidy` is found, we add a new `clang-tidy` build target:

```
# enable verbose output to see all warnings and errors
make VERBOSE=true clang-tidy
```

6.8 Extending PIConGPU

Section author: Sergei Bastrakov

Note: A number of places in *.param files* allow providing user-defined functors. The processing logic can largely be customized on that level, without modifying the source code. Such an external way is recommended when applicable. This section covers the case of extending the internal implementation.

6.8.1 General Simulation Loop Structure

A PIConGPU simulation effectively boils down to performing initialization and then executing a simulation loop. The simulation loop iterates over the requested number of time steps. For each time step, first all enabled plugins are called. Then all core computational stages are executed. Details of creating a new plugin or a new stage are presented below.

6.8.2 Adding a Plugin

PIConGPU plugins can perform computations or output, and often do both. Since all plugins are called at iteration start, they normally implement operations that are independent of the place in the computational loop. For operations requiring a specific ordering, please refer to the next section.

To add a new plugin, make a new file or subdirectory inside `include/picongpu/plugins`. Each plugin class must inherit our base class `ISimulationPlugin`. In turn, it largely uses its own base class `pmacc::ISimulationPlugin`. These classes define the interface of all PIConGPU plugins. The methods that most plugins want to override are:

- `pluginRegisterHelp()` adds command-line options for the plugin. In case a plugin introduces some new compile-time parameters, they are normally put to a new `.param` file.
- `pluginGetName()` sets a text name for the plugin, used to report errors currently.
- `pluginLoad()` initializes internal data of the plugin after the command-line arguments are submitted. Note that a constructor of the plugin class would be called before that and so often cannot do a full initialization. Is called once upon simulation start.
- `pluginUnload()` finalizes internal data if necessary, is called once at the end of the simulation.
- `setMappingDescription()` is used to pass simulation data to be used in kernels
- `notify()` runs the plugin for the given time iteration. This method implements the computational logic of the plugin. It often involves calling an internal algorithm or writing an own kernel. Those are described in the following sections.
- `checkpoint()` saves plugin internal data for checkpointing if necessary
- `restart()` loads the internal data from a checkpoint (necessary if `checkpoint()` writes some data)

Most plugins are run with a certain period in time steps. In this case, `Environment<>::get().PluginConnector().setNotificationPeriod(this, notifyPeriod)` can be used inside `pluginLoad()` to set this period. Then `notify()` will only be called for the active time steps.

For plugins (and most PIConGPU code) dealing with particles, it is common to template-parametrize based on species. Such plugins should use base class `plugins::multi::IInstance`. There is also a helper class `plugins::multi::IHelp` for command-line parameters prefixed for species. To match a plugin to applicable species, partially specialize trait `particles::traits::SpeciesEligibleForSolver`.

Regardless of the base class used, the new plugin class must be instantiated at `picongpu::PluginController` and the new headers included there. In case the plugin is conditionally available (e.g. requires an optional dependency), guards must also be placed there, around the include and instantiation.

When adding a plugin, do not forget to extend the documentation with plugin description and parameters. At least, extend the list of *plugins* and *command-line parameters* (the latter via `TBG_macros.cfg`). Other welcome additions for a new plugin include a dedicated documentation, a new example demonstrating usage in a realistic scenario, and a Python postprocessing script.

6.8.3 Adding a Simulation Stage

The currently executed simulation stages and their order are defined inside `Simulation::runOneStep()`. All stage classes are in `namespace picongpu::simulation::stage` and their implementations are located in respective directory. The existing stages share compatible interface and thus follow a pseudo-concept, not formally defined currently. The interface is also compatible to functors passed to `InitPipeline` and `IterationStartPipeline`. Note that stage classes are just wrappers around the internal implementations. Their purpose is to offer a high-level view of the steps and data dependencies in the computational loop, and add command-line parameters if necessary.

To add a new simulation stage:

- create a new `.hpp` file in `picongpu/simulation/stage`.
- write your stage functor class following the interface of other stage functors.
- if needed (e.g. for command-line parameters or static data) store an instance of it as a member of `Simulation` class.
- add a call to it inside `Simulation::runOneStep()`.

As mentioned above, a simulation stage should merely be calling an actual implementation located at an appropriate place inside PIConGPU or pmacc. When possible, it is recommended to use existing generic algorithms like `particles::Manipulate<>` or `FieldTmp::computeValue()`. Otherwise, one often has to implement an own kernel.

6.8.4 Writing a Kernel

Computational kernels are written using library cupla which is a layer on top of library alpaka. Most kernel functors are templates parametrized with the number of threads per block, often called `numWorkers`. Kernel invocations are wrapped into a helper macro `PMACC_KERNEL`.

A vast majority of PIConGPU kernels operate on two levels of parallelism: between supercells and inside each supercell. This parallel pattern is covered by the mapper concept.

template<uint32_t **`T_areaType`**, template<unsigned, typename> class **`T_MappingDescription`**, unsigned **`T_dim`**, typename
`class MapperConcept` : **`public`** *T_MappingDescription*<*T_dim*, *T_SupercellSize*>

Concept for mapper from block indices to supercells in the given area for alpaka kernels.

The mapping covers the case of supercell-level parallelism between alpaka blocks. The supercells can be processed concurrently in any order. This class is not used directly, but defines a concept for such mappers.

Mapper provides a 1:1 mapping from supercells in the area to alpaka blocks. (Since it is 1:1, the mapping is invertible, but only this direction is provided.) Dimensionality of the area indices and block indices is the same. A kernel must be launched with exactly getGridDim() blocks. Each block must process a single supercell with index getSuperCellIndex(blockIndex). Implementation is optimized for the standard areas in AreaType.

In-block parallelism is independent of this mapping and is done by a kernel. Naturally, this parallelism should also define block size, again independent of this mapping.

This pattern is used in most kernels in particle-mesh codes. Two most common parallel patterns are:

- for particle or particle-grid operations: alpaka block per supercell with this mapping, thread-level parallelism between particles of a frame
- for grid operations: alpaka block per supercell with this mapping, thread-level parallelism between cells of a supercell

Template Parameters

- `T_areaType`: parameter describing area to be mapped (depends on mapper type)
- `T_MappingDescription`: mapping description type, base class for *MapperConcept*
- `T_dim`: dimensionality of area and block indices
- `T_SupercellSize`: compile-time supercell size

For this parallel pattern, a mapper object provides the number of blocks to use for a kernel. On the device side, the object provides a mapping between alpaka blocks and supercells to be processed. Parallelism for threads between blocks is done inside the kernel. It is often over cells in a supercell or particles in a frame using *lockstep programming*.

A kernel often takes one or several data boxes from the host side. The data boxes allow array-like access to data. A more detailed description of boxes and other widely used classes is given in the following sections.

6.9 Important PIConGPU Classes

This is very, very small selection of classes of interest to get you started.

6.9.1 Simulation

`class Simulation` : **`public`** *pmacc*::SimulationHelper<*simDim*>

Global simulation controller class.

Initialises simulation data and defines the simulation steps for each iteration.

Template Parameters

- `DIM`: the dimension (2-3) for the simulation

Public Functions

`Simulation`()
Constructor.

void **`pluginRegisterHelp`**(po::options_description &*desc*)
Register command line parameters for this plugin.

Parameters are parsed and set prior to plugin load.

Parameters

- `desc`: boost::program_options description

std::string **`pluginGetName`**() **`const`**
Return the name of this plugin for status messages.

Return plugin name

void **`pluginLoad`**()

void **`pluginUnload`**()

void **`notify`**(uint32_t *currentStep*)
Notification callback.

For example Plugins can set their requested notification frequency at the PluginConnector

Parameters

- `currentStep`: current simulation iteration step

void **`init`**()
Initialize simulation.

Does hardware selections/reservations, memory allocations and initializes data structures as empty.

uint32_t **`fillSimulation`**()
Fills simulation with initial data after *init()*

Return returns the first step of the simulation (can be >0 for, e.g., restarts from checkpoints)

void **`runOneStep`**(uint32_t *currentStep*)
Run one simulation step.

Parameters

- `currentStep`: iteration number of the current step

void **`movingWindowCheck`**(uint32_t *currentStep*)
Check if moving window work must do.

If no moving window is needed the implementation of this function can be empty

Parameters

- `currentStep`: simulation step

void **resetAll** (uint32_t *currentStep*)
Reset the simulation to a state such as it was after *init()* but for a specific time step.

Can be used to call *fillSimulation()* again.

void **slide** (uint32_t *currentStep*)

virtual void **setInitController** (IInitPlugin **initController*)

MappingDesc ***getMappingDescription** ()

6.9.2 FieldE

class FieldE : **public** *picongpu*::*fields*::EMFieldBase<*FieldE*>
Representation of the electric field.

Stores field values on host and device and provides data synchronization between them.

Implements interfaces defined by *SimulationFieldHelper< MappingDesc >* and ISimulationData.

6.9.3 FieldB

class FieldB : **public** *picongpu*::*fields*::EMFieldBase<*FieldB*>
Representation of the magnetic field.

Stores field values on host and device and provides data synchronization between them.

Implements interfaces defined by *SimulationFieldHelper< MappingDesc >* and ISimulationData.

6.9.4 FieldJ

class FieldJ : **public** *pmacc*::SimulationFieldHelper<*MappingDesc*>, **public** *pmacc*::ISimulationData
Representation of the current density field.

Stores field values on host and device and provides data synchronization between them.

Implements interfaces defined by *SimulationFieldHelper< MappingDesc >* and ISimulationData.

6.9.5 FieldTmp

class FieldTmp : **public** *pmacc*::SimulationFieldHelper<*MappingDesc*>, **public** *pmacc*::ISimulationData
Representation of the temporary scalar field for plugins and temporary particle data mapped to grid (charge density, energy density, etc.)

Stores field values on host and device and provides data synchronization between them.

Implements interfaces defined by *SimulationFieldHelper< MappingDesc >* and ISimulationData.

6.9.6 Particles

template<typename **T_Name**, typename **T_Flags**, typename **T_Attributes**>
class Particles : **public** *pmacc*::ParticlesBase<ParticleDescription<*T_Name*, *SuperCellSize*, *T_Attributes*, *T_Flags*, bmpl
particle species

Template Parameters

- `T_Name`: name of the species [type boost::mpl::string]
- `T_Attributes`: sequence with attributes [type boost::mpl forward sequence]
- `T_Flags`: sequence with flags e.g. solver [type boost::mpl forward sequence]

Public Types

template<>
using SpeciesParticleDescription = *pmacc*::*ParticleDescription*<T_Name, *SuperCellSize*, T_Attributes, T_Fla

template<>
using ParticlesBaseType = ParticlesBase<*SpeciesParticleDescription*, *picongpu*::*MappingDesc*, *DeviceHeap*>

template<>
using FrameType = **typename** *ParticlesBaseType*::FrameType

template<>
using FrameTypeBorder = **typename** *ParticlesBaseType*::FrameTypeBorder

template<>
using ParticlesBoxType = **typename** *ParticlesBaseType*::ParticlesBoxType

Public Functions

Particles(**const** std::shared_ptr<*DeviceHeap*> &*heap*, *picongpu*::*MappingDesc cellDescription*, SimulationDataId *datasetID*)

void **createParticleBuffer**()

void **update**(uint32_t **const** *currentStep*)
Push all particles.

template<typename **T_MapperFactory**>
void **shiftBetweenSupercells**(*T_MapperFactory* **const** &*mapperFactory*, bool *onlyProcessMustShiftSupercells*)
Update the supercell storage for particles in the area according to particle attributes.

Template Parameters

- `T_MapperFactory`: factory type to construct a mapper that defines the area to process

Parameters

- `mapperFactory`: factory instance
- `onlyProcessMustShiftSupercells`: whether to process only supercells with mustShift set to true (optimization to be used with particle pusher) or process all supercells

void **applyBoundary**(uint32_t **const** *currentStep*)
Apply all boundary conditions.

template<typename **T_DensityFunctor**, typename **T_PositionFunctor**>
void **initDensityProfile**(*T_DensityFunctor* &*densityFunctor*, *T_PositionFunctor* &*positionFunctor*, **const** uint32_t *currentStep*)

template<typename **T_SrcName**, typename **T_SrcAttributes**, typename **T_SrcFlags**, typename **T_ManipulateF**
void **deviceDeriveFrom**(Particles<*T_SrcName*, *T_SrcAttributes*, *T_SrcFlags*> &*src*, *T_ManipulateFunctor* &*manipulateFunctor*, *T_SrcFilterFunctor* &*srcFilterFunctor*)

SimulationDataId **getUniqueId**()
Return the globally unique identifier for this simulation data.

Return globally unique identifier

void **synchronize**()
Synchronizes simulation data, meaning accessing (host side) data will return up-to-date values.

void **syncToDevice**()
Synchronize data from host to device.

template<typename **T_Pusher**>
void **push**(uint32_t **const** *currentStep*)
Do the particle push stage using the given pusher.

Template Parameters

- `T_Pusher`: non-composite pusher type

Parameters

- `currentStep`: current time iteration

Public Static Functions

static std::array<*particles*::boundary::Description, *simDim*> &**boundaryDescription**()
Get boundary descriptions for the species.

For both sides along the same axis, both boundaries have the same description. Must not be modified outside of the ParticleBoundaries simulation stage.

This method is static as it is used by static getStringProperties().

static *pmacc*::traits::StringProperty **getStringProperties**()

6.9.7 ComputeGridValuePerFrame

template<class **T_ParticleShape**, class **T_DerivedAttribute**>
class ComputeGridValuePerFrame

Public Types

template<>
using AssignmentFunction = **typename** T_ParticleShape::ChargeAssignment

template<>
using LowerMargin = **typename** *pmacc*::math::CT::make_Int<*simDim*, lowerMargin>::type

template<>
using UpperMargin = **typename** *pmacc*::math::CT::make_Int<*simDim*, upperMargin>::type

Public Functions

HDINLINE **ComputeGridValuePerFrame**()

HDINLINE float1_64 picongpu::particles::particleToGrid::ComputeGridValuePerFrame::ge
return unit for this solver

Return solver unit

HINLINE std::vector< float_64 > picongpu::particles::particleToGrid::ComputeGridValu
return powers of the 7 base measures for this solver

characterizing the unit of the result of the solver in SI (length L, mass M, time T, electric current I, thermodynamic temperature theta, amount of substance N, luminous intensity J)

template<typename FrameType, typename TVecSuperCell, typename BoxTmp, typename T_Acc

Public Static Functions

HINLINE std::string picongpu::particles::particleToGrid::ComputeGridValuePerFrame::g
return name of the this solver

Return name of solver

Public Static Attributes

constexpr int **supp** = AssignmentFunction::support

constexpr int **lowerMargin** = *supp* / 2

constexpr int **upperMargin** = (*supp* + 1) / 2

6.10 Important pmacc Classes

This is very, very small selection of classes of interest to get you started.

Note: Please help adding more Doxygen doc strings to the classes described below. As an example, here is a listing of possible extensive docs that new developers find are missing: https://github.com/ComputationalRadiationPhysics/picongpu/issues/776

6.10.1 Environment

template<uint32_t **T_dim**>
class Environment : **public** *pmacc*::detail::Environment
Global *Environment* singleton for PMacc.

Public Functions

void **enableMpiDirect**()

bool **isMpiDirectEnabled**() **const**

pmacc::GridController<T_dim> &**GridController**()
get the singleton GridController

Return instance of GridController

pmacc::SubGrid<T_dim> &**SubGrid**()
get the singleton SubGrid

Return instance of SubGrid

pmacc::Filesystem<T_dim> &**Filesystem**()
get the singleton Filesystem

Return instance of Filesystem

void **initDevices**(DataSpace<T_dim> *devices*, DataSpace<T_dim> *periodic*)
create and initialize the environment of PMacc

Usage of MPI or device(accelerator) function calls before this method are not allowed.

Parameters

- `devices`: number of devices per simulation dimension
- `periodic`: periodicity each simulation dimension (0 == not periodic, 1 == periodic)

void **initGrids**(DataSpace<T_dim> *globalDomainSize*, DataSpace<T_dim> *localDomainSize*, DataSpace<T_dim> *localDomainOffset*)
initialize the computing domain information of PMacc

Parameters

- `globalDomainSize`: size of the global simulation domain [cells]
- `localDomainSize`: size of the local simulation domain [cells]
- `localDomainOffset`: local domain offset [cells]

Environment(**const** *Environment*&)

Environment &**operator=**(**const** Environment&)

Public Static Functions

static Environment<T_dim> &**get**()
get the singleton Environment< DIM >

Return instance of Environment<DIM >

6.10.2 DataConnector

class DataConnector
Singleton class which collects and shares simulation data.

All members are kept as shared pointers, which allows their factories to be destroyed after sharing ownership with our *DataConnector*.

Public Functions

bool **hasId**(SimulationDataId *id*)
Returns if data with identifier id is shared.

Return if dataset with id is registered

Parameters

- `id`: id of the Dataset to query

void **initialise**(AbstractInitialiser &*initialiser*, uint32_t *currentStep*)
Initialises all Datasets using initialiser.

After initialising, the Datasets will be invalid.

Parameters

- `initialiser`: class used for initialising Datasets
- `currentStep`: current simulation step

void **share**(**const** std::shared_ptr<ISimulationData> &*data*)
Register a new Dataset and share its ownership.

If a Dataset with the same id already exists, a runtime_error is thrown. (Check with *DataConnector::hasId* when necessary.)

Parameters

- `data`: simulation data to share ownership

void **consume**(std::unique_ptr<ISimulationData> *data*)
Register a new Dataset and transfer its ownership.

If a Dataset with the same id already exists, a runtime_error is thrown. (Check with *DataConnector::hasId* when necessary.) The only difference from *share()* is transfer of ownership.

Parameters

- `data`: simulation data to transfer ownership

void **deregister**(SimulationDataId *id*)
End sharing a dataset with identifier id.

Parameters

- `id`: id of the dataset to remove

void **clean**()
Unshare all associated datasets.

template<class **TYPE**>
std::shared_ptr<*TYPE*> **get**(SimulationDataId *id*, bool *noSync* = false)
Returns shared pointer to managed data.

Reference to data in Dataset with identifier id and type TYPE is returned. If the Dataset status in invalid, it is automatically synchronized. Increments the reference counter to the dataset specified by id.

Return returns a reference to the data of type TYPE

Template Parameters

- `TYPE`: if of the data to load

Parameters

- `id`: id of the Dataset to load from
- `noSync`: indicates that no synchronization should be performed, regardless of dataset status

Friends

friend pmacc::DataConnector::detail::Environment

6.10.3 DataSpace

template<unsigned **T_Dim**>

class DataSpace : **public** *pmacc*::math::Vector<int, *T_Dim*>

A T_Dim-dimensional data space.

DataSpace describes a T_Dim-dimensional data space with a specific size for each dimension. It only describes the space and does not hold any actual data.

Template Parameters

- `T_Dim`: dimension (1-3) of the dataspace

Public Types

template<>
using BaseType = math::Vector<int, T_Dim>

Public Functions

HDINLINE **DataSpace**()

default constructor.

Sets size of all dimensions to 0.

constexpr HDINLINE DataSpace& pmacc::DataSpace::operator=(const DataSpace &)

HDINLINE **DataSpace**(cupla::dim3 *value*)

constructor.

Sets size of all dimensions from cuda dim3.

HDINLINE **DataSpace**(cupla::uint3 *value*)

constructor.

Sets size of all dimensions from cupla uint3 (e.g. cupla::threadIdx(acc)/cupla::blockIdx(acc))

HDINLINE **DataSpace**(**const** *DataSpace*<T_Dim> &*value*)

HDINLINE **DataSpace**(int *x*)

Constructor for DIM1-dimensional *DataSpace*.

Parameters

- `x`: size of first dimension

HDINLINE **DataSpace**(int *x*, int *y*)

Constructor for DIM2-dimensional *DataSpace*.

Parameters

- `x`: size of first dimension
- `y`: size of second dimension

HDINLINE **DataSpace**(int *x*, int *y*, int *z*)

Constructor for DIM3-dimensional *DataSpace*.

Parameters

- `x`: size of first dimension
- `y`: size of second dimension
- `z`: size of third dimension

HDINLINE **DataSpace**(**const** BaseType &*vec*)

HDINLINE **DataSpace**(**const** math::Size_t<T_Dim> &*vec*)

HDINLINE int pmacc::DataSpace::getDim() const
Returns number of dimensions (T_Dim) of this *DataSpace*.

Return number of dimensions

HINLINE bool pmacc::DataSpace::isOneDimensionGreaterThan(const DataSpace < T_Dim >
Evaluates if one dimension is greater than the respective dimension of other.

Return true if one dimension is greater, false otherwise

Parameters

- `other`: *DataSpace* to compare with

HDINLINE **operator math::Size_t<T_Dim>**() **const**

HDINLINE **operator cupla::dim3**() **const**

Public Static Functions

static HDINLINE DataSpace<T_Dim> pmacc::DataSpace::create(int value = 1)
Give *DataSpace* where all dimensions set to init value.

Return the new *DataSpace*

Parameters

- `value`: value which is setfor all dimensions

Public Static Attributes

constexpr int **Dim** = T_Dim

6.10.4 Vector

Warning: doxygenclass: Cannot find class "pmacc::math::Vector" in doxygen xml output for project "PIConGPU" from directory: ../xml

6.10.5 SuperCell

template<class **T_FrameType**>
class SuperCell

Public Functions

HDINLINE **SuperCell**()

HDINLINE T_FrameType* pmacc::SuperCell::FirstFramePtr()

HDINLINE T_FrameType* pmacc::SuperCell::LastFramePtr()

HDINLINE T_FrameType const* pmacc::SuperCell::FirstFramePtr() const

HDINLINE T_FrameType const* pmacc::SuperCell::LastFramePtr() const

HDINLINE bool pmacc::SuperCell::mustShift() const

HDINLINE void pmacc::SuperCell::setMustShift(bool const value)

HDINLINE uint32_t pmacc::SuperCell::getSizeLastFrame() const

HDINLINE uint32_t pmacc::SuperCell::getNumParticles() const

HDINLINE void pmacc::SuperCell::setNumParticles(uint32_t const size)

PMACC_ALIGN(firstFramePtr, T_FrameType *)

PMACC_ALIGN(lastFramePtr, T_FrameType *)

6.10.6 GridBuffer

template<class **TYPE**, unsigned **DIM**, class **BORDERTYPE** = *TYPE*>
class GridBuffer : **public** *pmacc*::HostDeviceBuffer<*TYPE*, *DIM*>

GridBuffer represents a DIM-dimensional buffer which exists on the host as well as on the device.

GridBuffer combines a HostBuffer and a DeviceBuffer with equal sizes. Additionally, it allows sending data from and receiving data to these buffers. Buffers consist of core data which may be surrounded by border data.

Template Parameters

- `TYPE`: datatype for internal Host- and DeviceBuffer
- `DIM`: dimension of the buffers
- `BORDERTYPE`: optional type for border data in the buffers. TYPE is used by default.

Public Types

template<>
using DataBoxType = **typename** Parent::DataBoxType

Public Functions

GridBuffer(**const** GridLayout<DIM> &*gridLayout*, bool *sizeOnDevice* = false)

Constructor.

Parameters

- `gridLayout`: layout of the buffers, including border-cells
- `sizeOnDevice`: if true, size information exists on device, too.

GridBuffer(**const** DataSpace<DIM> &*dataSpace*, bool *sizeOnDevice* = false)

Constructor.

Parameters

- `dataSpace`: *DataSpace* representing buffer size without border-cells
- `sizeOnDevice`: if true, internal buffers must store their size additionally on the device (as we keep this information coherent with the host, it influences performance on host-device copies, but some algorithms on the device might need to know the size of the buffer)

GridBuffer(DeviceBuffer<TYPE, DIM> &*otherDeviceBuffer*, **const** GridLayout<DIM> &*gridLayout*, bool *sizeOnDevice* = false)

Constructor.

Parameters

- `otherDeviceBuffer`: DeviceBuffer which should be used instead of creating own DeviceBuffer
- `gridLayout`: layout of the buffers, including border-cells
- `sizeOnDevice`: if true, internal buffers must store their size additionally on the device (as we keep this information coherent with the host, it influences performance on host-device copies, but some algorithms on the device might need to know the size of the buffer)

GridBuffer(HostBuffer<TYPE, DIM> &*otherHostBuffer*, **const** DataSpace<DIM> &*offsetHost*, DeviceBuffer<TYPE, DIM> &*otherDeviceBuffer*, **const** DataSpace<DIM> &*offsetDevice*, **const** GridLayout<DIM> &*gridLayout*, bool *sizeOnDevice* = false)

void **addExchange**(uint32_t *dataPlace*, **const** Mask &*receive*, DataSpace<DIM> *guardingCells*, uint32_t *communicationTag*, bool *sizeOnDeviceSend*, bool *sizeOnDeviceReceive*)

Add Exchange in *GridBuffer* memory space.

An Exchange is added to this *GridBuffer*. The exchange buffers use the same memory as this *GridBuffer*.

Parameters

- `dataPlace`: place where received data is stored [GUARD | BORDER] if dataPlace=GUARD than copy other BORDER to my GUARD if dataPlace=BORDER than copy other GUARD to my BORDER
- `receive`: a Mask which describes the directions for the exchange
- `guardingCells`: number of guarding cells in each dimension
- `communicationTag`: unique tag/id for communication has to be the same when this method is called multiple times for the same object (with non-overlapping masks)
- `sizeOnDeviceSend`: if true, internal send buffers must store their size additionally on the device (as we keep this information coherent with the host, it influences performance on host-device copies, but some algorithms on the device might need to know the size of the buffer)
- `sizeOnDeviceReceive`: if true, internal receive buffers must store their size additionally on the device

void **addExchange**(uint32_t *dataPlace*, **const** Mask &*receive*, DataSpace<DIM> *guardingCells*, uint32_t *communicationTag*, bool *sizeOnDevice* = false)

Add Exchange in *GridBuffer* memory space.

An Exchange is added to this *GridBuffer*. The exchange buffers use the same memory as this *GridBuffer*.

Parameters

- `dataPlace`: place where received data is stored [GUARD | BORDER] if dataPlace=GUARD than copy other BORDER to my GUARD if dataPlace=BORDER than copy other GUARD to my BORDER
- `receive`: a Mask which describes the directions for the exchange
- `guardingCells`: number of guarding cells in each dimension
- `communicationTag`: unique tag/id for communication
- `sizeOnDevice`: if true, internal buffers must store their size additionally on the device (as we keep this information coherent with the host, it influences performance on host-device copies, but some algorithms on the device might need to know the size of the buffer)

void **addExchangeBuffer**(**const** Mask *&receive*, **const** DataSpace<DIM> *&dataSpace*, uint32_t *communicationTag*, bool *sizeOnDeviceSend*, bool *sizeOnDeviceReceive*)

Add Exchange in dedicated memory space.

An Exchange is added to this *GridBuffer*. The exchange buffers use the their own memory instead of using the *GridBuffer*'s memory space.

Parameters

- `receive`: a Mask which describes the directions for the exchange
- `dataSpace`: size of the newly created exchange buffer in each dimension
- `communicationTag`: unique tag/id for communication
- `sizeOnDeviceSend`: if true, internal send buffers must store their size additionally on the device (as we keep this information coherent with the host, it influences performance on host-device copies, but some algorithms on the device might need to know the size of the buffer)
- `sizeOnDeviceReceive`: if true, internal receive buffers must store their size additionally on the device

void **addExchangeBuffer**(**const** Mask *&receive*, **const** DataSpace<DIM> *&dataSpace*, uint32_t *communicationTag*, bool *sizeOnDevice* = false)

Add Exchange in dedicated memory space.

An Exchange is added to this *GridBuffer*. The exchange buffers use the their own memory instead of using the *GridBuffer*'s memory space.

Parameters

- `receive`: a Mask which describes the directions for the exchange
- `dataSpace`: size of the newly created exchange buffer in each dimension
- `communicationTag`: unique tag/id for communication
- `sizeOnDevice`: if true, internal buffers must store their size additionally on the device (as we keep this information coherent with the host, it influences performance on host-device copies, but some algorithms on the device might need to know the size of the buffer)

bool **hasSendExchange**(uint32_t *ex*) **const**

Returns whether this *GridBuffer* has an Exchange for sending in ex direction.

Return true if send exchanges with ex direction exist, otherwise false

Parameters

- `ex`: exchange direction to query

bool **hasReceiveExchange**(uint32_t *ex*) **const**

Returns whether this *GridBuffer* has an Exchange for receiving from ex direction.

Return true if receive exchanges with ex direction exist, otherwise false

Parameters

- `ex`: exchange direction to query

Exchange<BORDERTYPE, DIM> &**getSendExchange**(uint32_t *ex*) **const**

Returns the Exchange for sending data in ex direction.

Returns an Exchange which for sending data from this *GridBuffer* in the direction described by ex.

Return the Exchange for sending data

Parameters

- `ex`: the direction to query

Exchange<BORDERTYPE, DIM> &**getReceiveExchange**(uint32_t *ex*) **const**
Returns the Exchange for receiving data from ex direction.

Returns an Exchange which for receiving data to this *GridBuffer* from the direction described by ex.

Return the Exchange for receiving data

Parameters

- `ex`: the direction to query

Mask **getSendMask**() **const**
Returns the Mask describing send exchanges.

Return Mask for send exchanges

Mask **getReceiveMask**() **const**
Returns the Mask describing receive exchanges.

Return Mask for receive exchanges

EventTask **communication**()
Starts sync data from own device buffer to neighbor device buffer.

Asynchronously starts synchronization data from internal DeviceBuffer using added Exchange buffers. This operation runs sequential to other code but intern asynchronous

EventTask **asyncCommunication**(EventTask *serialEvent*)
Starts sync data from own device buffer to neighbor device buffer.

Asynchronously starts synchronization data from internal DeviceBuffer using added Exchange buffers.

EventTask **asyncSend**(EventTask *serialEvent*, uint32_t *sendEx*)

EventTask **asyncReceive**(EventTask *serialEvent*, uint32_t *recvEx*)

GridLayout<DIM> **getGridLayout**()
Returns the GridLayout describing this *GridBuffer*.

Return the layout of this buffer

Protected Attributes

bool **hasOneExchange**

uint32_t **lastUsedCommunicationTag**

GridLayout<DIM> **gridLayout**

Mask **sendMask**

Mask **receiveMask**

template<>
std::unique_ptr<ExchangeIntern<BORDERTYPE, DIM>> **sendExchanges**[27]

template<>

std::unique_ptr<ExchangeIntern<BORDERTYPE, DIM>> **receiveExchanges**[27]

template<>
EventTask **receiveEvents**[27]

template<>
EventTask **sendEvents**[27]

uint32_t **maxExchange**

6.10.7 SimulationFieldHelper

template<class **CellDescription**>
class SimulationFieldHelper

Public Types

template<>
using MappingDesc = CellDescription

Public Functions

SimulationFieldHelper(CellDescription *description*)

virtual ~SimulationFieldHelper()

virtual void **reset**(uint32_t *currentStep*) = 0
Reset is as well used for init.

virtual void **syncToDevice**() = 0
Synchronize data from host to device.

CellDescription **getCellDescription**() **const**

Protected Attributes

CellDescription **cellDescription**

6.10.8 ParticlesBase

template<typename **T_ParticleDescription**, class **T_MappingDesc**, typename **T_DeviceHeap**>
class ParticlesBase : **public** *pmacc*::SimulationFieldHelper<*T_MappingDesc*>

Public Types

enum [anonymous]
Values:

Dim = MappingDesc::Dim

Exchanges = traits::NumberOfExchanges<*Dim*>::value

TileSize = math::CT::volume<**typename** MappingDesc::SuperCellSize>::type::value

template<>
using BufferType = ParticlesBuffer<*ParticleDescription*, **typename** MappingDesc::SuperCellSize, T_DeviceHeap, M

template<>

using FrameType = **typename** *BufferType*::FrameType

template<>
using FrameTypeBorder = **typename** *BufferType*::FrameTypeBorder

template<>
using ParticlesBoxType = **typename** *BufferType*::ParticlesBoxType

template<>
using HandleGuardRegion = **typename** *ParticleDescription*::HandleGuardRegion

template<>
using SimulationDataTag = ParticlesTag

Public Functions

template<typename **T_MapperFactory**>
void **fillGaps**(*T_MapperFactory* **const** &*mapperFactory*)
Fill gaps in an area defined by a mapper factory.

Template Parameters

- `T_MapperFactory`: factory type to construct a mapper that defines the area to process

Parameters

- `mapperFactory`: factory instance

void **fillAllGaps**()

void **fillBorderGaps**()

void **deleteGuardParticles**(uint32_t *exchangeType*)

template<uint32_t **T_area**>
void **deleteParticlesInArea**()

void **copyGuardToExchange**(uint32_t *exchangeType*)
copy guard particles to intermediate exchange buffer

Copy all particles from the guard of a direction to the device exchange buffer.

Warning This method resets the number of particles in the processed supercells even if there are particles left in the supercell and does not guarantee that the last frame is contiguous filled. Call fillAllGaps afterwards if you need a valid number of particles and a contiguously filled last frame.

void **insertParticles**(uint32_t *exchangeType*)

ParticlesBoxType **getDeviceParticlesBox**()

ParticlesBoxType **getHostParticlesBox**(**const** int64_t *memoryOffset*)

BufferType &**getParticlesBuffer**()

void **reset**(uint32_t *currentStep*)
Reset is as well used for init.

Protected Functions

ParticlesBase(**const** std::shared_ptr<T_DeviceHeap> &*deviceHeap*, MappingDesc *description*)

~ParticlesBase()

template<uint32_t **T_area**>
void **shiftParticles**(bool *onlyProcessMustShiftSupercells*)

Shift all particles in an area defined by a mapper factory.

The factory type must be such that StrideMapperFactory<T_MapperFactory, stride> is specialized

Parameters

- `onlyProcessMustShiftSupercells`: whether to process only supercells with mustShift set to true (optimization to be used with particle pusher) or process all supercells

template<typename **T_MapperFactory**>
void **shiftParticles**(*T_MapperFactory* **const** &*mapperFactory*, bool *onlyProcessMustShiftSupercells*)

Shift all particles in the area defined by the given factory.

Note that the area itself is not strided, but the factory must produce stride mappers for the area.

Template Parameters

- `T_strideMapperFactory`: factory type to construct a stride mapper, resulting mapper must have stride of at least 3, adheres to the MapperFactory concept

Parameters

- `mapperFactory`: factory instance
- `onlyProcessMustShiftSupercells`: whether to process only supercells with mustShift set to true (optimization to be used with particle pusher) or process all supercells

Protected Attributes

BufferType ***particlesBuffer**

6.10.9 ParticleDescription

template<typename **T_Name**, typename **T_SuperCellSize**, typename **T_ValueTypeSeq**, typename **T_Flags** = bmpl::vect
struct ParticleDescription

ParticleDescription defines attributes, methods and flags of a particle.

This class holds no runtime data. The class holds information about the name, attributes, flags and methods of a particle.

Template Parameters

- `T_Name`: name of described particle (e.g. electron, ion) type must be a boost::mpl::string
- `T_SuperCellSize`: compile time size of a super cell
- `T_ValueTypeSeq`: sequence or single type with value_identifier
- `T_Flags`: sequence or single type with identifier to add flags on a frame
- `T_MethodsList`: sequence or single class with particle methods (e.g. calculate mass, gamma, . . .) (e.g. useSolverXY, calcRadiation, . . .)

- `T_FrameExtensionList`: sequence or single class with frame extensions
  - extension must be an unary template class that supports bmpl::apply1<>
  - type of the final frame is applied to each extension class (this allows pointers and references to a frame itself)
  - the final frame that uses *ParticleDescription* inherits from all extension classes

Public Types

template<>
using Name = T_Name

template<>
using SuperCellSize = T_SuperCellSize

template<>
using ValueTypeSeq = **typename** ToSeq<T_ValueTypeSeq>::type

template<>
using FlagsList = **typename** ToSeq<T_Flags>::type

template<>
using HandleGuardRegion = T_HandleGuardRegion

template<>
using MethodsList = **typename** ToSeq<T_MethodsList>::type

template<>
using FrameExtensionList = **typename** ToSeq<T_FrameExtensionList>::type

template<>
using ThisType = ParticleDescription<*Name*, *SuperCellSize*, *ValueTypeSeq*, *FlagsList*, *HandleGuardRegion*, *MethodsLi*

6.10.10 ParticleBox

Warning: doxygenstruct: Cannot find class "pmacc::ParticlesBox" in doxygen xml output for project "PIConGPU" from directory: ../xml

6.10.11 Frame

template<typename **T_CreatePairOperator**, typename **T_ParticleDescription**>
struct Frame : **public** *pmacc*::InheritLinearly<*T_ParticleDescription*::MethodsList>, **protected** *pmacc*::math::MapTuple
Frame is a storage for arbitrary number >0 of Particles with attributes.

See MapTupel

Template Parameters

- `T_CreatePairOperator`: unary template operator to create a boost pair from single type (pair<name,dataType>)

Template Parameters

- `T_ValueTypeSeq`: sequence with value_identifier
- `T_MethodsList`: sequence of classes with particle methods (e.g. calculate mass, gamma, ...)
- `T_Flags`: sequence with identifiers to add flags on a frame (e.g. useSolverXY, calcRadiation, ...)

Public Types

template<>
using ParticleDescription = T_ParticleDescription

template<>
using Name = **typename** *ParticleDescription*::Name

template<>
using SuperCellSize = **typename** *ParticleDescription*::SuperCellSize

template<>
using ValueTypeSeq = **typename** *ParticleDescription*::ValueTypeSeq

template<>
using MethodsList = **typename** *ParticleDescription*::MethodsList

template<>
using FlagList = **typename** *ParticleDescription*::FlagsList

template<>
using FrameExtensionList = **typename** *ParticleDescription*::FrameExtensionList

template<>
using ThisType = Frame<T_CreatePairOperator, *ParticleDescription*>

template<>
using BaseType = pmath::MapTuple<**typename** SeqToMap<*ValueTypeSeq*, T_CreatePairOperator>::type, pmath::Alig

template<>
using ParticleType = *pmacc*::Particle<*ThisType*>

Public Functions

HDINLINE ParticleType pmacc::Frame::operator[](const uint32_t idx)
access the Nth particle

HDINLINE const ParticleType pmacc::Frame::operator[](const uint32_t idx) const
access the Nth particle

template<typename T_Key>HDINLINE auto& pmacc::Frame::getIdentifier(const T_Key)
access attribute with a identifier

Return result of operator[] of MapTupel

Parameters

- `T_Key`: instance of identifier type (can be an alias, value_identifier or any other class)

template<typename T_Key>HDINLINE const auto& pmacc::Frame::getIdentifier(const T_Key
const version of method *getIdentifier(const T_Key)*

Public Static Functions

static HINLINE std::string pmacc::Frame::getName()

6.10.12 IPlugin

class IPlugin : **public** *pmacc*::INotify
Subclassed by picongpu::ISimulationPlugin, picongpu::ISimulationStarter, *pmacc::SimulationHelper< DIM >*, *pmacc::SimulationHelper< simDim >*

Public Functions

IPlugin()

~IPlugin()

virtual void **load**()

virtual void **unload**()

bool **isLoaded**()

virtual void **checkpoint**(uint32_t *currentStep*, **const** std::string *checkpointDirectory*) = 0
Notifies plugins that a (restartable) checkpoint should be created for this timestep.

Parameters

- `currentStep`: cuurent simulation iteration step
- `checkpointDirectory`: common directory for checkpoints

virtual void **restart**(uint32_t *restartStep*, **const** std::string *restartDirectory*) = 0
Restart notification callback.

Parameters

- `restartStep`: simulation iteration step to restart from
- `restartDirectory`: common restart directory (contains checkpoints)

virtual void **pluginRegisterHelp**(po::options_description &*desc*) = 0
Register command line parameters for this plugin.

Parameters are parsed and set prior to plugin load.

Parameters

- `desc`: boost::program_options description

virtual std::string **pluginGetName**() **const** = 0
Return the name of this plugin for status messages.

Return plugin name

virtual void **onParticleLeave**(**const** std::string&, **const** int32_t)
Called each timestep if particles are leaving the global simulation volume.

This method is only called for species which are marked with the `GuardHandlerCallPlugins` policy in their descpription.

The order in which the plugins are called is undefined, so this means read-only access to the particles.

Parameters

- `speciesName`: name of the particle species
- `direction`: the direction the particles are leaving the simulation

uint32_t **getLastCheckpoint**() **const**
When was the plugin checkpointed last?

Return last checkpoint's time step

void **setLastCheckpoint**(uint32_t *currentStep*)
Remember last checkpoint call.

Parameters

- `currentStep`: current simulation iteration step

Protected Functions

virtual void **pluginLoad**()

virtual void **pluginUnload**()

Protected Attributes

bool **loaded** = {false}

uint32_t **lastCheckpoint** = {0}

6.10.13 PluginConnector

class PluginConnector
Plugin registration and management class.

Public Functions

void **registerPlugin**(*IPlugin* **plugin*)
Register a plugin for loading/unloading and notifications.

Plugins are loaded in the order they are registered and unloaded in reverse order. To trigger plugin notifications, call

See *setNotificationPeriod* after registration.

Parameters

- `plugin`: plugin to register

void **loadPlugins**()
Calls load on all registered, not loaded plugins.

void **unloadPlugins**()
Unloads all registered, loaded plugins.

std::list<po::options_description> **registerHelp**()
Publishes command line parameters for registered plugins.

Return list of boost program_options command line parameters

void **setNotificationPeriod**(INotify **notifiedObj*, std::string **const** &*period*)
Set the notification period.

Parameters

- `notifiedObj`: the object to notify, e.g. an *IPlugin* instance
- `period`: notification period

void **notifyPlugins**(uint32_t *currentStep*)
Notifies plugins that data should be dumped.

Parameters

- `currentStep`: current simulation iteration step

void **checkpointPlugins**(uint32_t *currentStep*, **const** std::string *checkpointDirectory*)
Notifies plugins that a restartable checkpoint should be dumped.

Parameters

- `currentStep`: current simulation iteration step
- `checkpointDirectory`: common directory for checkpoints

void **restartPlugins**(uint32_t *restartStep*, **const** std::string *restartDirectory*)
Notifies plugins that a restart is required.

Parameters

- `restartStep`: simulation iteration to restart from
- `restartDirectory`: common restart directory (contains checkpoints)

template<typename **Plugin**>
std::vector<*Plugin* *> **getPluginsFromType**()
Get a vector of pointers of all registered plugin instances of a given type.

Return vector of plugin pointers

Template Parameters

- `Plugin`: type of plugin

std::list<*IPlugin* *> **getAllPlugins**() **const**
Return a copied list of pointers to all registered plugins.

Friends

friend pmacc::PluginConnector::detail::Environment

6.10.14 SimulationHelper

template<unsigned **DIM**>
class SimulationHelper : **public** *pmacc*::*IPlugin*
Abstract base class for simulations.

Use this helper class to write your own concrete simulations by binding pure virtual methods.

Template Parameters

- `DIM`: base dimension for the simulation (2-3)

Public Types

template<>
using SeqOfTimeSlices = std::vector<pluginSystem::TimeSlice>

Public Functions

SimulationHelper()
Constructor.

~SimulationHelper()

virtual void **runOneStep**(uint32_t *currentStep*) = 0
Must describe one iteration (step).

This function is called automatically.

virtual void **init**() = 0
Initialize simulation.

Does hardware selections/reservations, memory allocations and initializes data structures as empty.

virtual uint32_t **fillSimulation**() = 0
Fills simulation with initial data after *init()*

Return returns the first step of the simulation (can be >0 for, e.g., restarts from checkpoints)

virtual void **resetAll**(uint32_t *currentStep*) = 0
Reset the simulation to a state such as it was after *init()* but for a specific time step.

Can be used to call *fillSimulation()* again.

virtual void **movingWindowCheck**(uint32_t *currentStep*) = 0
Check if moving window work must do.

If no moving window is needed the implementation of this function can be empty

Parameters

- `currentStep`: simulation step

void **notifyPlugins**(uint32_t *currentStep*)
Call all plugins.

This function is called inside the simulation loop.

Parameters

- `currentStep`: simulation step

virtual void **dumpOneStep**(uint32_t *currentStep*)
Write a checkpoint if needed for the given step.

This function is called inside the simulation loop.

Parameters

- `currentStep`: simulation step

GridController<DIM> &**getGridController**()

void **dumpTimes**(TimeIntervall &*tSimCalculation*, TimeIntervall&, double &*roundAvg*, uint32_t *currentStep*)

void **startSimulation**()
Begin the simulation.

void **pluginRegisterHelp**(po::options_description &*desc*)
Register command line parameters for this plugin.

Parameters are parsed and set prior to plugin load.

Parameters

- `desc`: boost::program_options description

std::string **pluginGetName**() **const**
Return the name of this plugin for status messages.

Return plugin name

void **pluginLoad**()

void **pluginUnload**()

void **restart**(uint32_t *restartStep*, **const** std::string *restartDirectory*)
Restart notification callback.

Parameters

- `restartStep`: simulation iteration step to restart from
- `restartDirectory`: common restart directory (contains checkpoints)

void **checkpoint**(uint32_t *currentStep*, **const** std::string *checkpointDirectory*)
Notifies plugins that a (restartable) checkpoint should be created for this timestep.

Parameters

- `currentStep`: cuurent simulation iteration step
- `checkpointDirectory`: common directory for checkpoints

Protected Functions

std::vector<uint32_t> **readCheckpointMasterFile**()
Reads the checkpoint master file if any and returns all found checkpoint steps.

Return vector of found checkpoints steps in order they appear in the file

Protected Attributes

uint32_t **runSteps** = {0}

uint32_t **softRestarts**
Presentations: loop the whole simulation `softRestarts` times from initial step to runSteps.

std::string **checkpointPeriod**

SeqOfTimeSlices **seqCheckpointPeriod**

std::string **checkpointDirectory**

uint32_t **numCheckpoints** = {0}

int32_t **restartStep** = {-1}

std::string **restartDirectory**

bool **restartRequested** = {false}

const std::string **CHECKPOINT_MASTER_FILE**

std::string **author**

bool **useMpiDirect** = {false}
enable MPI gpu direct

bool **tryRestart** = false

6.10.15 ForEach

Warning: doxygenstruct: Cannot find class "meta::ForEach" in doxygen xml output for project "PIConGPU" from directory: ../xml

6.10.16 Kernel Start

template<typename **T_KernelFunctor**>
struct Kernel
wrapper for the user kernel functor

contains debug information like filename and line of the kernel call

Public Types

template<>
using KernelType = T_KernelFunctor

Public Functions

HINLINE **Kernel**(T_KernelFunctor **const** &*kernelFunctor*, std::string **const** &*file* = std::string(), size_t **const** *line* = 0)

Return

Parameters

- `gridExtent`: grid extent configuration for the kernel
- `blockExtent`: block extent configuration for the kernel
- `sharedMemByte`: dynamic shared memory used by the kernel (in byte)

template<typename T_VectorGrid, typename T_VectorBlock>HINLINE auto pmacc::exec::Ker
configured kernel object

this objects contains the functor and the starting parameter

Template Parameters

- `T_VectorGrid`: type which defines the grid extents (type must be castable to cupla dim3)
- `T_VectorBlock`: type which defines the block extents (type must be castable to cupla dim3)

Parameters

- `gridExtent`: grid extent configuration for the kernel
- `blockExtent`: block extent configuration for the kernel
- `sharedMemByte`: dynamic shared memory used by the kernel (in byte)

Public Members

T_KernelFunctor **const m_kernelFunctor**
functor

std::string **const m_file**
file name from where the kernel is called

size_t **const m_line**
line number in the file

PMACC_KERNEL(...)
create a kernel object out of a functor instance

this macro add the current filename and line number to the kernel object

Parameters

- ...: instance of kernel functor

6.10.17 Struct Factory

Syntax to generate structs with all members inline. Allows to conveniently switch between variable and constant defined members without the need to declare or initialize them externally. See for example PIConGPU's *density.param* for usage.

PMACC_STRUCT(name, ...)
generate a struct with static and dynamic members

```
PMACC_STRUCT(StructAlice,
    // constant member variable
    (PMACC_C_VALUE(float, varFoo, -1.0))
    // lvalue member variable
    (PMACC_VALUE(float, varFoo, -1.0))
    // constant vector member variable
    (PMACC_C_VECTOR_DIM(double, 3, vectorBarC, 1.134e-5, 1.134e-5, 1.134e-5))
    // lvalue vector member variable
    (PMACC_VECTOR_DIM(double, 3, vectorBarC, 1.134e-5, 1.134e-5, 1.134e-5))
    // constant string member variable
    (PMACC_C_STRING(someString, "anythingYouWant: even spaces!"))
    // plain C++ member
    PMACC_EXTENT(
        using float_64 = double;
        static constexpr int varBar = 42;
    );
);
```

Note do not forget the surrounding parenthesize for each element of a sequence

Parameters

- name: name of the struct
- ...: preprocessor sequence with TypeMemberPair's e.g. (*PMACC_C_VALUE(int,a,2)*)

PMACC_C_VECTOR_DIM(type, dim, name, ...)
create static const member vector that needs no memory inside of the struct

```
PMACC_C_VECTOR_DIM(float_64, simDim, center_SI, 1.134e-5, 1.134e-5, 1.134e-5);
// is syntactically equivalent to
static const Vector<float_64,simDim> center_SI = Vector<float_64,simDim>(1.
↪134e-5, 1.134e-5, 1.134e-5);
```

Parameters

- `type`: type of an element
- `dim`: number of vector components
- `name`: member variable name
- `...`: enumeration of init values (number of components must be greater or equal than dim)

PMACC_C_VALUE(type, name, value)
create static constexpr member

```
PMACC_C_VALUE(float_64, power_SI, 2.0);
// is syntactically equivalent to
static constexpr float_64 power_SI = float_64(2.0);
```

Parameters

- `type`: type of the member
- `name`: member variable name
- `value`: init value

PMACC_VALUE(type, name, initValue)
create changeable member

```
PMACC_VALUE(float_64, power_SI, 2.0);
// is the equivalent of
float_64 power_SI(2.0);
```

Parameters

- `type`: type of the member
- `name`: member variable name
- `value`: init value

PMACC_VECTOR(type, name, ...)
create changeable member vector

```
PMACC_VECTOR(float2_64, center_SI, 1.134e-5, 1.134e-5);
// is the equivalent of
float2_64 center_SI(1.134e-5, 1.134e-5);
```

Parameters

- `type`: type of an element
- `name`: member variable name
- `...`: enumeration of init values

PMACC_VECTOR_DIM(type, dim, name, ...)
create changeable member vector

```
PMACC_VECTOR_DIM(float_64, simDim, center_SI, 1.134e-5, 1.134e-5, 1.134e-5);
// is the equivalent of
Vector<float_64,3> center_SI(1.134e-5, 1.134e-5, 1.134e-5);
```

Parameters

- `type`: type of an element

- `dim`: number of vector components
- `name`: member variable name
- `...`: enumeration of init values (number of components must be equal to dim)

PMACC_C_STRING (name, initValue)
create static const character string

```
PMACC_C_STRING(filename, "fooFile.txt");
// is syntactically equivalent to
static const char* filename = (char*)"fooFile.txt";
```

Parameters

- `name`: member variable name
- `char_string`: character string

PMACC_EXTENT (...)
create any code extension

```
PMACC_EXTENT(typedef float FooFloat;)
// is the equivalent of
typedef float FooFloat;
```

Parameters

- `...`: any code

6.10.18 Identifier

Construct unique types, e.g. to name, access and assign default values to particle species' attributes. See for example PIConGPU's speciesAttributes.param for usage.

value_identifier (in_type, name, in_default)
define a unique identifier with name, type and a default value

The created identifier has the following options: getValue() - return the user defined value getName() - return the name of the identifier ::type - get type of the value

Parameters

- `in_type`: type of the value
- `name`: name of identifier
- `in_value`: user defined value of in_type (can be a constructor of a class)

e.g. value_identifier(float,length,0.0f) typedef length::type value_type; // is float value_type x = length::getValue(); //set x to 0.f printf("Identifier name: %s",length::getName()); //print Identifier name: length

to create a instance of this value_identifier you can use: `length()` or `length_`

alias (name)
create an alias

an alias is a unspecialized type of an identifier or a value_identifier

example: alias(aliasName); //create type varname

Parameters

- `name`: name of alias

to specialize an alias do: aliasName<valueIdentifierName> to create an instance of this alias you can use: aliasName(); or aliasName_

get type which is represented by the alias typedef typename traits::Resolve<name>::type resolved_type;

6.11 Python Postprocessing Tool Structure

Each plugin should implement at least the following Python classes.

1. A data reader class responsible for loading the data from the simulation directory
2. A visualizer class that outputs a matplotlib plot
3. A jupyter-widget class that exposes the parameters of the matplotlib visualizer to the user via other widgets.

The repository directory for PIConGPU Python modules for plugins is `lib/python/picongpu/plugins/`.

6.11.1 Data Reader

The data readers should reside in the `lib/python/picongpu/plugins/data` directory. There is a base class in `base_reader.py` defining the interface of a reader. Each reader class should derive from this class and implement the interface functions not implemented in this class.

To shorten the import statements for the readers, please also add an entry in the `__init__.py` file of the `data` directory.

6.11.2 Matplotlib visualizer

The visualizers should reside in the `lib/python/picongpu/plugins/plot_mpl/` directory. The module names should end on `_visualizer.py` and the class name should only be `Visualizer`.

To shorten the import statements for the visualizers, please also add an entry in the `__init__.py` file of the `plot_mpl` directory with an alias that ends on "MPL".

There is a base class for visualization found in `base_visualizer.py` which already handles the plotting logic. It uses (possibly multiple) instances of the data reader classes for accessing the data. Visualizing data simultaneously for more than one scan is supported by creating as many readers and plot objects as there are simulations for visualization. After getting the data, it ensures that (for performance reasons) a matplotlib artist is created only for the first plot and later only gets updated with fresh data.

All new plugins should derive from this class.

When implementing a new visualizer you have to perform the following steps:

1. Let your visualizer class inherit from the `Visualizer` class in `base visualizer.py` and call the base class constructor with the correct data reader class.

2. Implement the `_create_plt_obj(self, idx)` function. This function needs to access the plotting data from the `self.data` member (this is the data structure as returned by the data readers `.get(...)` function, create some kind of matplotlib artist by storing it in the `self.plt_obj` member variable at the correct index specified by the idx variable (which corresponds to the data of the simulation at position idx that is passed in construction.

3. Implement the `_update_plt_obj(self, idx)` function. This is called only after a valid `self.plt_obj` was created. It updates the matplotlib artist with new data. Therefore it again needs to access the plotting data from the `self.data` member and call the data update API for the matplotlib artist (normally via `.set_data(...)`.

6.11.3 Jupyter Widget

The widget is essentially only a wrapper around the matplotlib visualizer that allows dynamical adjustment of the parameters the visualizer accepts for plotting. This allows to adjust e.g. species, filter and other plugin-dependent options without having to write new lines of Python code.

The widgets should reside in the `lib/python/picongpu/plugins/jupyter_widgets/` directory. The module names should end on `_widget.py`.

To shorten the import statements for the widgets, please also add an entry in the `__init__.py` file of the `jupyter_widget` directory.

There is a base class for visualization found in `base_widget.py` which already handles most of the widget logic.

It allows to switch between visualizations for different simulation times (iterations) and different simulations.

When implementing a new widget you have to perform the following steps:

1. Let the widget class inherit from the `BaseWidget` class in `base_widget.py` and call the base class constructor with the correct matplotlib visualizer class.

```
from .base_widget import BaseWidget

class NewPluginWidget(BaseWidget):
```

2. In the constructor, call the base class constructor with the matplotlib visualizer class as `plot_mpl_cls` keyword.

   The base class will then create an instance of the visualizer class and delegate the plotting job to it.

```
# taken from lib/python/picongpu/plugins/jupyter_widgets/energy_histogram_widget.py
from .base_widget import BaseWidget
from picongpu.plugins.plot_mpl import EnergyHistogramMPL

class EnergyHistogramWidget(BaseWidget):
    def __init__(self, run_dir_options, fig=None, **kwargs):

        BaseWidget.__init__(self,
                            EnergyHistogramMPL,
                            run_dir_options,
                            fig,
                            **kwargs)
```

3. implement the `_create_widgets_for_vis_args(self)` function.

   This function has to define jupyter widgets as member variables of the class to allow interactive manipulation of parameters the underlying matplotlib visualizer is capable of handling. It needs to return a dictionary using the parameter names the matplotlib visualizer accepts as keys and the widget members that correspond to these parameters as values.

```
# taken from lib/python/picongpu/plugins/jupyter_widgets/energy_histogram_widget.py
 def _create_widgets_for_vis_args(self):
     # widgets for the input parameters
     self.species = widgets.Dropdown(description="Species",
                                     options=["e"],
                                     value='e')
     self.species_filter = widgets.Dropdown(description="Species_filter",
                                            options=['all'],
                                            value="all")

     return {'species': self.species,
             'species_filter': self.species_filter}
```

6.12 Debugging

Section author: Sergei Bastrakov

When investigating the reason of a crashing simulation, it is very helpful to reduce the setup as much as possible while the crash is still happening. This includes moving to fewer (and ideally to 1) MPI processes, having minimal grid size (ideally 3 supercells), disabling unrelated plugins and simulation stages. Such a reduction should be done incrementally while checking whether the issue is still observed. Knowing when the issue disappears could hint to its source. This process also significantly speeds up and helps to focus a following deeper look.

The following build options can assist the investigation:

- `PIC_VERBOSE=<N>` sets log detail level for PIConGPU, highest level is 127.
- `PMACC_VERBOSE=<N>` sets log detail level for pmacc, highest level is 127.
- `PMACC_BLOCKING_KERNEL=ON` makes each kernel invocation blocking, which helps to narrow a crash down to a particular kernel.
- `CUPLA_STREAM_ASYNC_ENABLE=OFF` disables asynchronous streams, also helps to narrow a crash down to a particular place.

These options can be passed when building, or manually modified via cmake. An example build command is

```
pic-build -c "-DPIC_VERBOSE=127 -DPMACC_VERBOSE=127 -DPMACC_BLOCKING_KERNEL=ON -
↪DCUPLA_STREAM_ASYNC_ENABLE=OFF"
```

When reporting a crash, it is helpful if you attached the output `stdout` and `stderr` of such a build.

For further debugging tips and use of tools please refer to our Wiki.

6.13 Index of Doxygen Documentation

This command is currently taking up to 2 GB of RAM, so we can't run it on read-the-docs:

doxygenindex::

project PIConGPU

path '../xml'

outline

no-link

CHAPTER

SEVEN

PROGRAMMING PATTERNS

See also:

In order to follow this section, you need to understand the CUDA programming model.

7.1 Lockstep Programming Model

Section author: René Widera, Axel Huebl

The *lockstep programming model* structures code that is evaluated collectively and independently by workers (physical threads). Actual processing is described by one-dimensional index domains of *virtual workers* which can even be changed within a kernel. Mathematically, index domains are none-injective, total functions on physical workers.

An index domain is **independent** from data but **can** be mapped to a data domain, e.g. one to one or with more complex mappings.

Code which is implemented by the *lockstep programming model* is free of any dependencies between the number of worker and processed data elements. To simplify the implementation, each index within a domain can be seen as a *virtual worker* which is processing one data element (like the common workflow to programming CUDA). Each *worker* i can be executed as N_i *virtual workers* $(1 : N_i)$.

Functors passed into lockstep routines can have three different parameter signatures.

- No parameter, if the work is not requiring the linear index within a domain: `[&](){ }`
- An unsigned 32bit integral parameter if the work depends on indices within the domain `range [0, domain size): [&](uint32_t const linearIdx){}`
- `lockstep::Idx` as parameter. lockstep::Idx is holing the linear index within the domain and meta information to access a context variables: `[&](pmacc::mappings::threads::lockstep::Idx const idx){}`

7.1.1 pmacc helpers

template<uint32_t **T_domainSize**, uint32_t **T_numWorkers**, uint32_t **T_simdSize**>
struct Config

describe a constant index domain

describe the size of the index domain and the number of workers to operate on a lockstep domain

Template Parameters

- `T_domainSize`: number of indices in the domain
- `T_numWorkers`: number of worker working on `T_domainSize`
- `T_simdSize`: SIMD width

Subclassed by pmacc::lockstep::ForEach< Config< T_domainSize, T_numWorkers, T_simdSize > >

struct Idx
Hold current index within a lockstep domain.

template<uint32_t **T_numWorkers**>
class Worker
holds a worker configuration

collection of the compile time number of workers and the runtime worker index

Template Parameters

- `T_numWorkers`: number of workers which are used to execute this functor

Subclassed by pmacc::lockstep::ForEach< Config< T_domainSize, T_numWorkers, T_simdSize > >

template<typename **T_Type**, typename **T_Config**>
struct Variable : **protected** *pmacc*::memory::Array<*T_Type*, *T_Config*::maxIndicesPerWorker>, **public** *T_Config*
Variable used by virtual worker.

This object is designed to hold context variables in lock step programming. A context variable is just a local variable of a virtual worker. Allocating and using a context variable allows to propagate virtual worker states over subsequent lock steps. A context variable for a set of virtual workers is owned by their (physical) worker.

Data stored in a context variable should only be used with a lockstep programming construct e.g. lockstep::ForEach<>

Warning: doxygenstruct: Cannot find class "pmacc::lockstep::ForEach" in doxygen xml output for project "PIConGPU" from directory: ../xml

7.1.2 Common Patterns

Create a Context Variable

A context variable is used to transfer information from a subsequent lockstep to another. You can use a context variable `lockstep::Variable`, similar to a temporary local variable in a function. A context variable must be defined outside of `ForEach` and should be accessed within the functor passed to `ForEach` only.

- ... and initialize with the index of the virtual worker

```
// assume one dimensional indexing of threads within a block
uint32_t const workerIdx = cupla::threadIdx(acc).x;
constexpr uint32_t frameSize = 256;
constexpr uint32_t numWorkers = 42;
auto forEachParticleSlotInFrame = lockstep::makeForEach<frameSize, numWorkers>
↪(workerIdx);
auto vIdx = forEachParticleSlotInFrame(
    [](lockstep::Idx const idx) -> int32_t
    {
        return idx;
    }
);

// is equal to

// assume one dimensional indexing of threads within a block
uint32_t const workerIdx = cupla::threadIdx(acc).x;
constexpr uint32_t frameSize = 256;
constexpr uint32_t numWorkers = 42;
auto forEachParticleSlotInFrame = lockstep::makeForEach<frameSize, numWorkers>
↪(workerIdx);
```

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```
// variable will be uninitialized
auto vIdx = lockstep::makeVar<int32_t>(forEachParticleSlotInFrame);
forEachParticleSlotInFrame(
    [&](lockstep::Idx const idx)
    {
        vIdx[idx] = idx;
    }
);
```

- To default initialize a context variable you can pass the arguments directly during the creation.

```
// assume one dimensional indexing of threads within a block
uint32_t const workerIdx = cupla::threadIdx(acc).x;
constexpr uint32_t frameSize = 256;
constexpr uint32_t numWorkers = 42;
auto forEachParticleSlotInFrame = lockstep::makeForEach<frameSize, numWorkers>
↪(workerIdx, 23);
```

- Data from a context variable can be accessed within independent lock steps. A virtual worker has only access to there own context variable data.

```
// assume one dimensional indexing of threads within a block
uint32_t const workerIdx = cupla::threadIdx(acc).x;
constexpr uint32_t frameSize = 256;
constexpr uint32_t numWorkers = 42;
auto forEachParticleSlotInFrame = lockstep::makeForEach<frameSize, numWorkers>
↪(workerIdx);
auto vIdx = forEachParticleSlotInFrame(
    [](lockstep::Idx const idx) -> int32_t
    {
        return idx;
    }
);

// store old linear index into oldVIdx
auto oldVIdx = forEachExample(
    [&](lockstep::Idx const idx) -> int32_t
    {
        int32_t old = vIdx[idx];
        printf("virtual worker linear idx: %u == %u\n", vIdx[idx], idx);
        vIdx[idx] += 256;
        return old;
    }
);

forEachExample(
    [&](lockstep::Idx const idx)
    {
        printf("nothing changed: %u == %u - 256 == %u\n", oldVIdx[idx], vIdx[idx],␣
↪idx);
    }
);
```

Collective Loop

- each worker needs to pass a loop N times
- in this example, there are more dates than workers that process them

```
// `frame` is a list which must be traversed collectively
while( frame.isValid() )
{
    // assume one dimensional indexing of threads within a block
    uint32_t const workerIdx = cupla::threadIdx(acc).x;
    constexpr uint32_t frameSize = 256;
    constexpr uint32_t numWorkers = 42;
    auto forEachParticleSlotInFrame = lockstep::makeForEach<frameSize, numWorkers>
↪(workerIdx);
    forEachParticleSlotInFrame(
       [&](lockstep::Idx const idx)
       {
           // independent work, idx can be used to access a context variable
       }
    forEachParticleSlotInFrame(
       [&](uint32_t const linearIdx)
       {
           // independent work based on the linear index only
       }
   );
}
```

Non-Collective Loop

- each *virtual worker* increments a private variable

```
// assume one dimensional indexing of threads within a block
uint32_t const workerIdx = cupla::threadIdx(acc).x;
constexpr uint32_t frameSize = 256;
constexpr uint32_t numWorkers = 42;
auto forEachParticleSlotInFrame = lockstep::makeForEach<frameSize, numWorkers>
↪(workerIdx);
auto vWorkerIdx = lockstep::makeVar<int32_t>(forEachParticleSlotInFrame, 0);
forEachParticleSlotInFrame(
    [&](auto const idx)
    {
        // assign the linear index to the virtual worker context variable
        vWorkerIdx[idx] = idx;
        for(int i = 0; i < 100; i++)
            vWorkerIdx[idx]++;
    }
);
```

Using a Master Worker

- only one *virtual worker* (called *master*) of all available `numWorkers` manipulates a shared data structure for all others

```
// example: allocate shared memory (uninitialized)
PMACC_SMEM(
    finished,
    bool
);

// assume one dimensional indexing of threads within a block
uint32_t const workerIdx = cupla::threadIdx(acc).x;
auto onlyMaster = lockstep::makeMaster(workerIdx);

// manipulate shared memory
```

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```
onlyMaster(
    [&]( )
    {
        finished = true;
    }
);

/* important: synchronize now, in case upcoming operations (with
 * other workers) access that manipulated shared memory section
 */
cupla::__syncthreads(acc);
```

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