CP2K Developers Meeting

2025/02/24

Topics

Part 1 CP2K Developers Meeting

– Best practices for development and contributions

– New and Ongoing Developments

– Current Issues with CP2K

– Next CP2K Release

– Planned Events in the Context of CP2K

Part 2 GPU-Development with CP2K

– Portable-CUDA Concept

– Other GPU Programming Topics

– ...

Part 1: CP2K Developers Meeting

Part 1: CP2K Developers Meeting

Best practices for development and contributions (HansP, MathieuT, OleS)

- Mandatory reviews
  - Currently, core developers are dispensed

PROs:	speed and ease of contribution; "no burden for real science"
CONs:	Dashboard may break; (mandatory tests are fine)

- More mandatory tests

PROs:	... More tests are better
CONs:	Higher cost (cloud)

Notes

- Opinions/thoughts?
  - Ole: common practise, but cost effort; not enough manpower to review every request
  - Hans/Ole: not really a shortage of reviews right now
  - Rocco: possibility to request reviews would be helpful
  - Ole: maybe for developers groups can be used
  - Ole: three tests automatically run (code formatting, sdbg) and are mandatory
  - Hans/Ole: reviewers/core developers can launch additional tests like parallel
  - Hans: maybe randomization
  - Ole: Google Cloud cost in the green again
  - Robert: maybe run tests on HPC
  - Ole: one CSCS test is up and running
  - Ole: github actions with HPC systems
  - **Policy: always add new tests for new functionalities/algorithms or major changes**

Migration from Makefile to CMake

What‘s left to do:

- libgrpp (PR 3966)
- Debug builds
- GPU builds
- Other architectures: ARM, macOS, (might drop i386)
- Exotic builds (coverage, conventions, sanitizers)

Roadmap:

- 2025.2 release: Declare Makefile as deprecated
- After 2025.2 release:
  - Remove Makefile from master branch
  - Remove DBCSR submodule
  - Simplify Toolchain
- 2026.1 release: Only ships with CMake

Migration from DBCSR to DBM

What‘s done:

- Dropped single precision matrices
- Dropped complex matrices
- Moved high level routines to cp_dbcsr_contrib.F

What‘s left to do:

- Maybe refactor cp_blacs_env to use Cartesian MPI Communicators.
- Maybe merge mp_cart_type with mp_comm_type.
- Implement symmetric matrices.
- Implement replication.
- Refactor arnoldi so we can drop dbcsr_get_data_p()
- Refactor hfx_energy_potential.F so we can drop dbcsr_dot_threadsafe().
- Implement reading/writting CSR files.
- Implement reading/writting our custom binary files.

New and Ongoing Developments in CP2K

Developments@CASUS

- Finite-Temperature Random Phase Approximation (Frederick)
  - testing/fixing in progress
- Migrate Multigrid code to C/GPU
  - Application for OpenHackathon@Jülich in April (Frederick, Johann, Jiři)
  - needs to write a new FFT backend (GPL vs BSD license)
- Tblite interface to the GFN2-xTB method (Johann)
- OpenPMD as alternative IO method for reading/writing cube files in CP2K (Franz)

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www.casus.science

Integrating openPMD output/input into CP2K

Current effort at adding openPMD-based data handling for natively-parallel binary output based on HDF5/ADIOS2 according to a F.A.I.R. scientific data standard

HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF

TECHNISCHE UNIVERSITÄT DRESDEN

CBG Max Planck Institute of Molecular Cell Biology and Genetics

HELMHOLTZ Centre for Environmental Research

Uniwersytet Wrocławski

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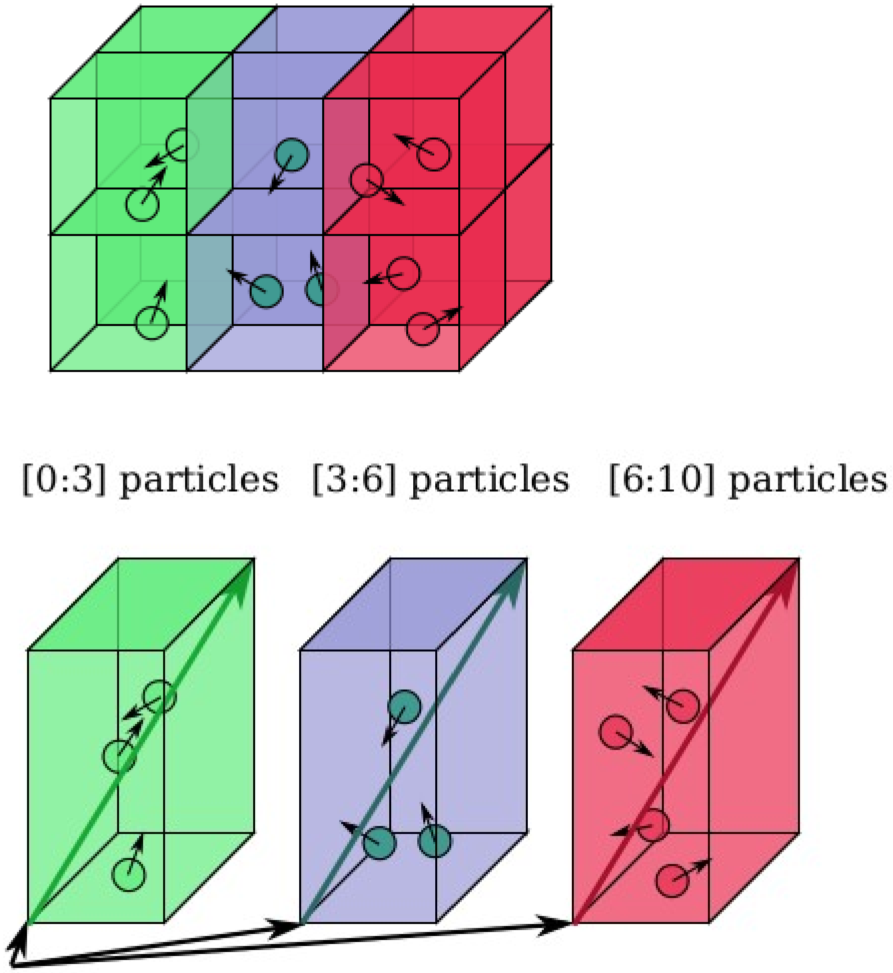
Freistaat SACHSEN

What is particle-mesh data?



Mesh

n-dimensional space,
divided into discrete cells

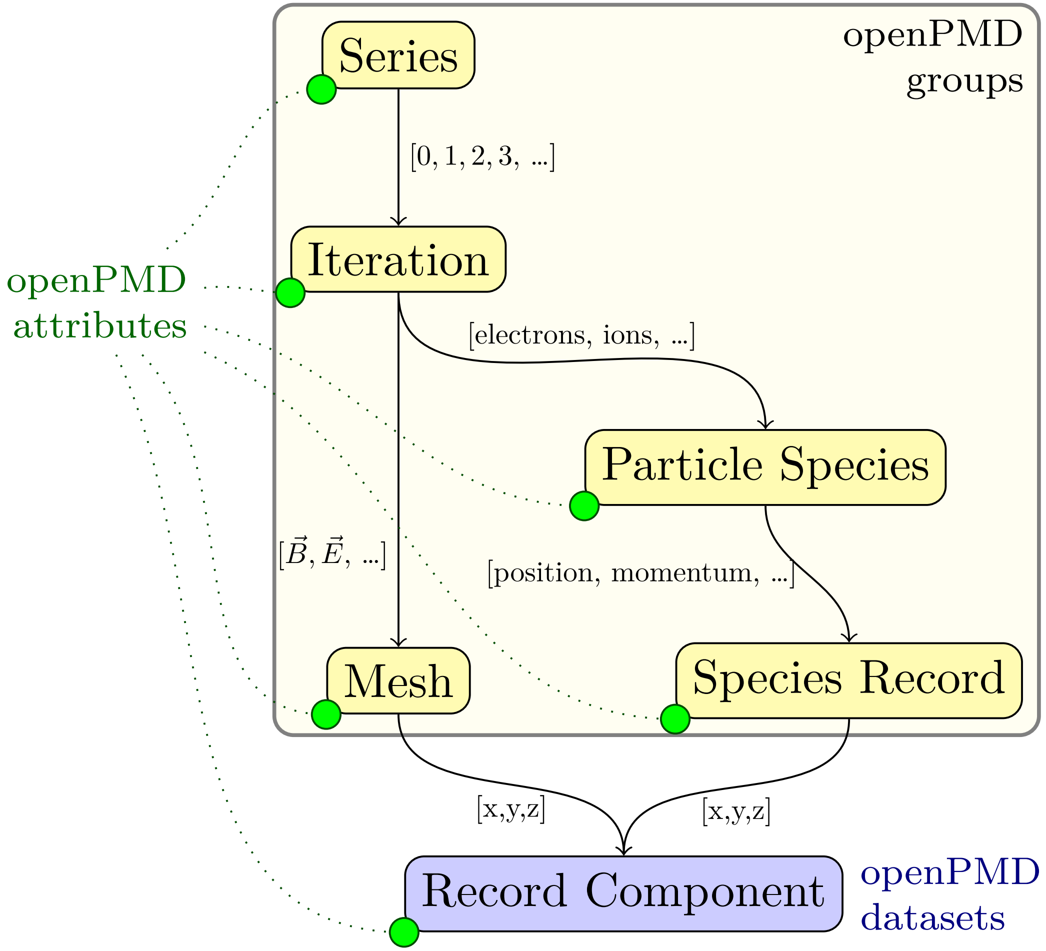
- e.g. temperature:
  store a scalar number per cell
- e.g. electrical fields:
  store a 3D vector per cell

Particles

A list of discrete objects,
located on the mesh

- for each particle: list its position
- optionally: list charge, weight, …

openPMD hierarchy

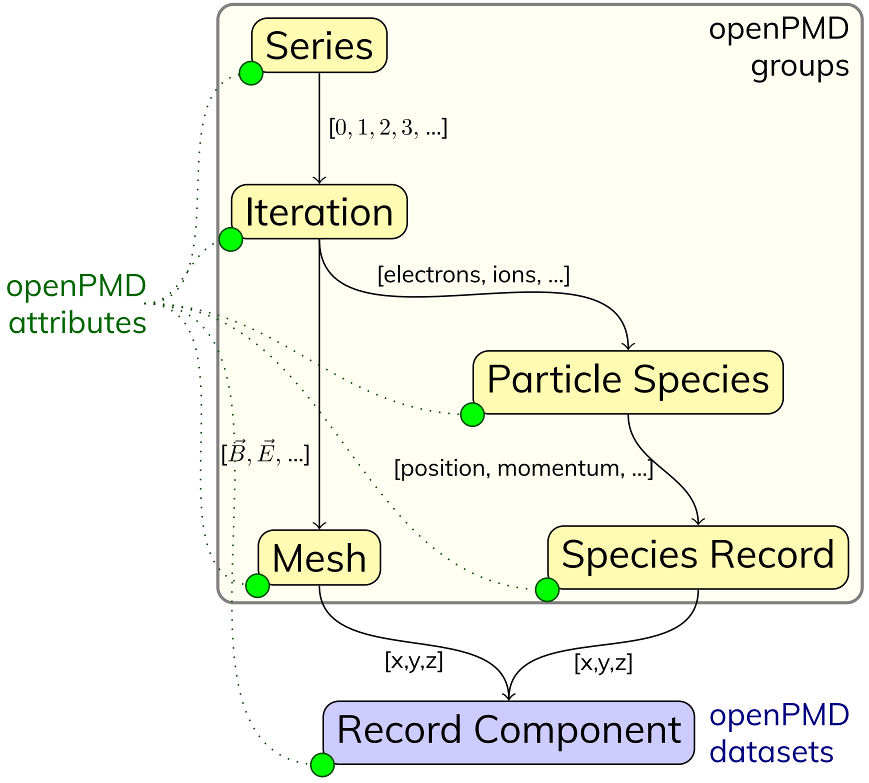


- **Structure** for series & snapshots encoded as either:
  - **files** (one file per iteration)
  - **groups** (reuse files)
  - **variables** (reuse files & variables in ADIOS2)

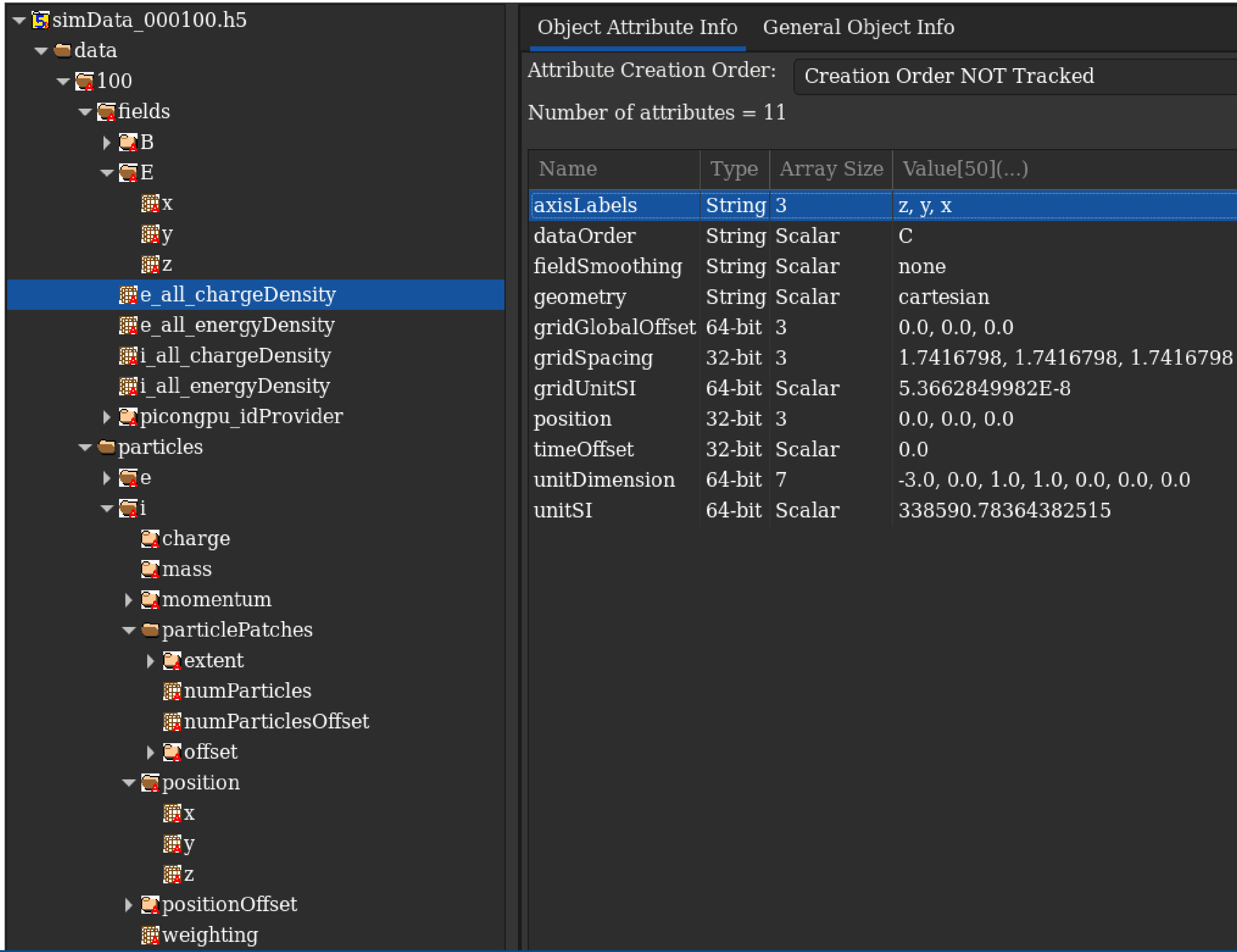
- Records for **physical observables**
  constants, mixed precision, complex numbers

- **Attributes:** unit conversion, description, relations, mesh geometry, authors, env. info, ...

Example dataset: HDF5 backend



Sample data created with PIConGPU



```
simData_000100.h5
  data
    100
      fields
        B
        E
          x
          y
          z
        e_all_chargeDensity
        e_all_energyDensity
        i_all_chargeDensity
        i_all_energyDensity
        picongpu_idProvider
      particles
        e
        i
          charge
          mass
          momentum
          particlePatches
            extent
            numParticles
            numParticlesOffset
            offset
          position
            x
            y
            z
          positionOffset
          weighting
```

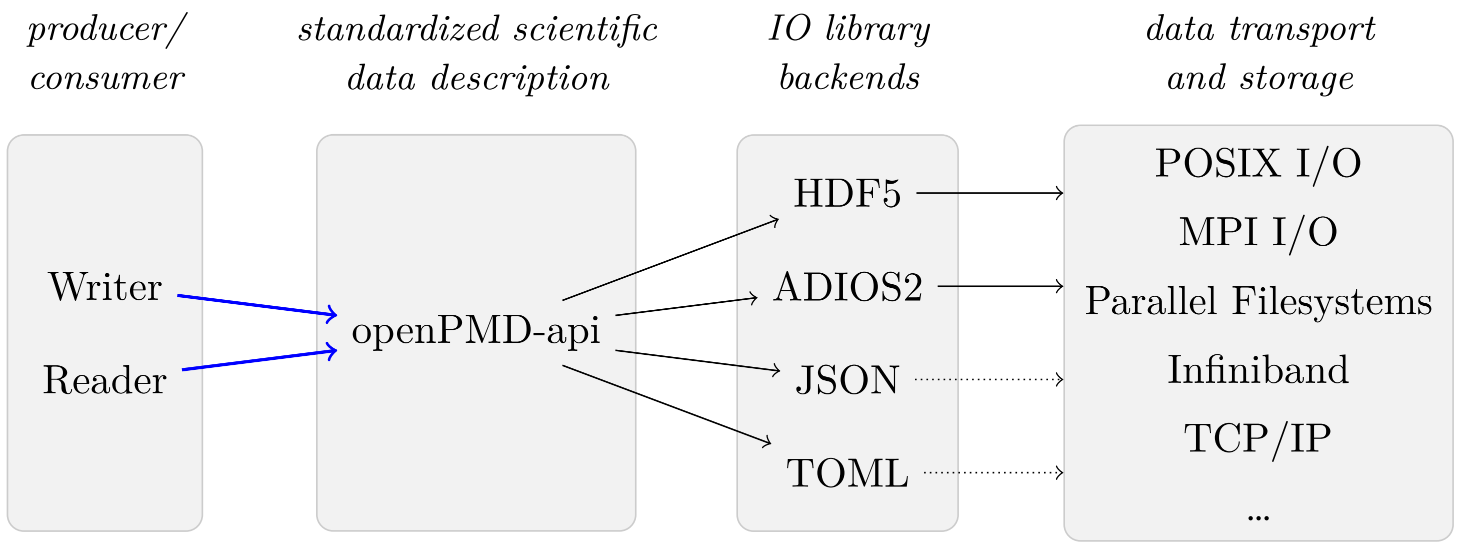
Object Attribute Info | General Object Info

Attribute Creation Order: Creation Order NOT Tracked

Number of attributes = 11

Name	Type	Array Size	Value[50](...)
axisLabels	String	3	z, y, x
dataOrder	String	Scalar	C
fieldSmoothing	String	Scalar	none
geometry	String	Scalar	cartesian
gridGlobalOffset	64-bit	3	0.0, 0.0, 0.0
gridSpacing	32-bit	3	1.7416798, 1.7416798, 1.7416798
gridUnitSI	64-bit	Scalar	5.3662849982E-8
position	32-bit	3	0.0, 0.0, 0.0
timeOffset	32-bit	Scalar	0.0
unitDimension	64-bit	7	-3.0, 0.0, 1.0, 1.0, 0.0, 0.0, 0.0
unitSI	64-bit	Scalar	338590.78364382515

openPMD-api – open stack for scientific I/O



producer/ consumer

standardized scientific data description

IO library backends

data transport and storage

Writer

Reader

openPMD-api

HDF5

ADIOS2

JSON

TOML

POSIX I/O

MPI I/O

Parallel Filesystems

Infiniband

TCP/IP

...

```python
import openpmd_api as io

# pick and configure backend via JSON/TOML or inferred from filename extension
adios_config = """
  backend = "adios2"
  [[adios2.dataset.operators]]
  type = "blosc" # activate compression
"""
mode = io.Access.create
series = io.Series("simOutput.h5",   mode
                   """{"hdf5": {"vfd": {"type": "subfiling"}}}""")
series = io.Series("simOutput.bp5",  mode, adios_config)
series = io.Series("simOutput.sst",  mode, "@./or/load/config/from/file.json")
series = io.Series("simOutput.json", mode)
```

- MPI support at all levels
- Implemented in C++17
- Bindings in C++17, Python and (dev version only) Julia
- Specify backend at runtime:
  I/O library, transport, compression, streaming, aggregation, …

Reference Implementation in C++ & Bindings: Python and Julia

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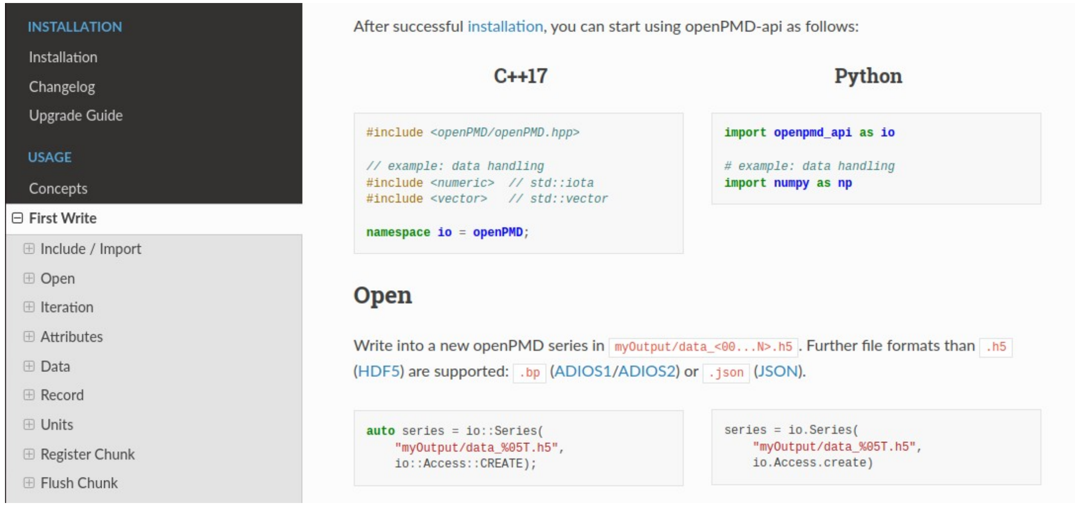
Online Documentation: openpmd-api.readthedocs.io



After successful installation, you can start using openPMD-api as follows:

C++17

```
#include <openPMD/openPMD.hpp>

// example: data handling
#include <numeric>  // std::iota
#include <vector>   // std::vector

namespace io = openPMD;
```

Python

```
import openpmd_api as io

# example: data handling
import numpy as np
```

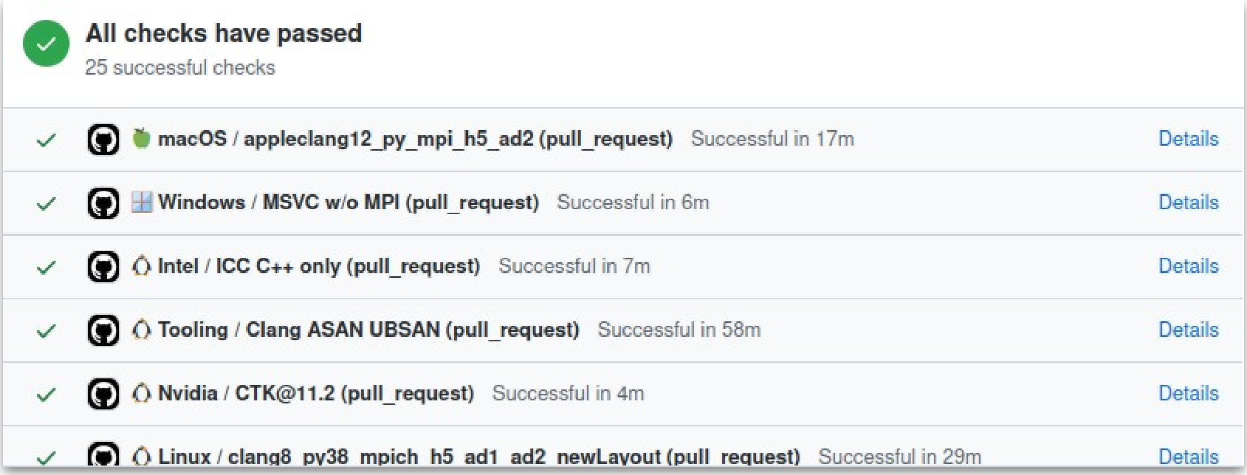
Open

Write into a new openPMD series in `myOutput/data_<00...N>.h5`. Further file formats than `.h5` (HDF5) are supported: `.bp` (ADIOS1/ADIOS2) or `.json` (JSON).

```
auto series = io::Series(
    "myOutput/data_%05T.h5",
    io::Access::CREATE);
```

```
series = io.Series(
    "myOutput/data_%05T.h5",
    io.Access.create)
```

Open-Source Development & Tests: github.com/openPMD/openPMD-api



All checks have passed
25 successful checks

✓ macOS / appleclang12_py_mpi_h5_ad2 (pull_request) Successful in 17m Details
✓ Windows / MSVC w/o MPI (pull_request) Successful in 6m Details
✓ Intel / ICC C++ only (pull_request) Successful in 7m Details
✓ Tooling / Clang ASAN UBSAN (pull_request) Successful in 58m Details
✓ Nvidia / CTK@11.2 (pull_request) Successful in 4m Details
✓ Linux / clang8_py38_mpich_h5_ad1_ad2_newLayout (pull_request) Successful in 29m Details

Rapid and easy installation on any platform:

```
python3 -m pip install
        openpmd-api
```

```
brew tap openpmd/openpmd
brew install openpmd-api
```

```
cmake -S . -B build
cmake --build build
    --target install
```

```
conda install
    -c conda-forge
    openpmd-api
```

```
spack install
      openpmd-api
```

```
module load openpmd-api
```

A Huebl, F Poeschel, F Koller, J Gu, et al.
"openPMD-api: C++ & Python API for Scientific I/O with openPMD" (2018) DOI:10.14278/rodare.27

openPMD powered Projects and Users

Documents:

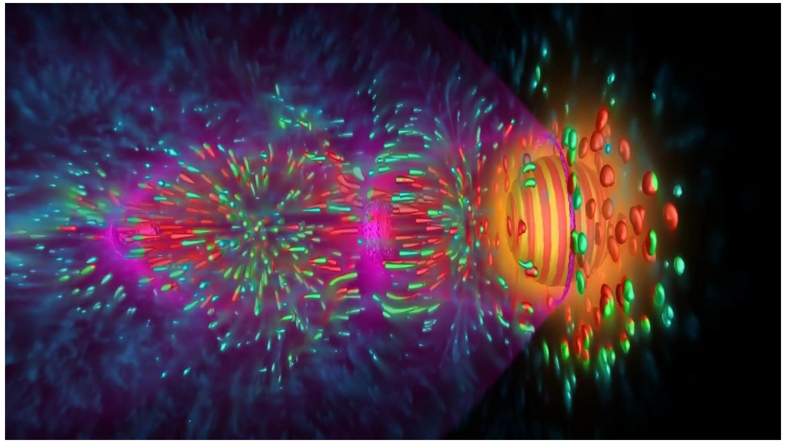
- **openPMD standard** (1.0.0, 1.0.1, 1.1.0)
  the underlying file markup and definition
  A Huebl et al., doi: 10.5281/zenodo.33624

Language Binding:

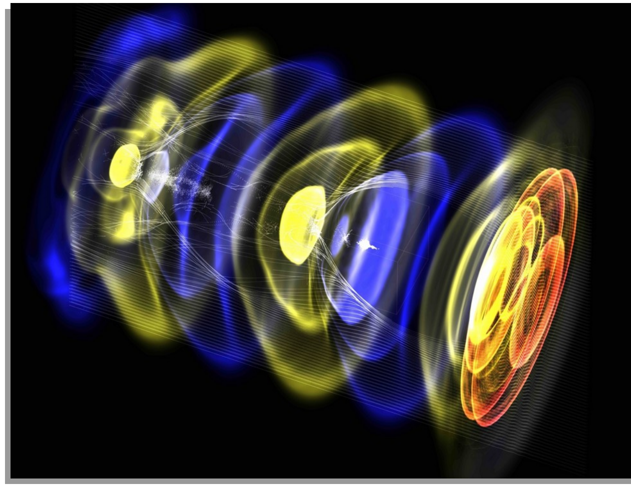
- **openPMD-api** (HZDR, CASUS, LBNL)
  reference API for openPMD data handling
  maintainers: A Huebl, J Gu, F Poeschel et al.

Scientific Simulations:

- **PIConGPU** (HZDR)
  electro-dynamic particle-in-cell code
  maintainers: R Widera, S Bastrakov, A Debus et al.
- **WarpX** (LBNL, LLNL)
  electro-dynamic/static particle-in-cell code
  maintainers: JL Vay, D Grote, R Lehe, A Huebl et al.
- **FBPIC** (LBNL, DESY)
  spectral, fourier-bessel particle-in-cell code
  maintainers: R Lehe, M Kirchen et al.
- **SimEx Platform** (EUCALL, European XFEL)
  simulation of advanced photon experiments
  maintainer: C Fortmann-Grote



PIConGPU+ISAAC on Summit
2nd prize Helmholtz Imaging
Best Scientific Image Contest 2022
Image credit: Felix Meyer/HZDR



WarpX
PI: Jean-Luc Vay/LBNL

see also: https://github.com/openPMD/openPMD-projects

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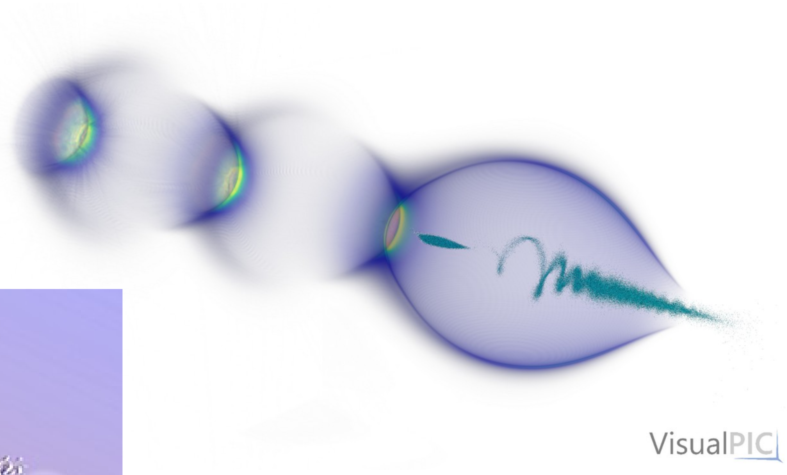
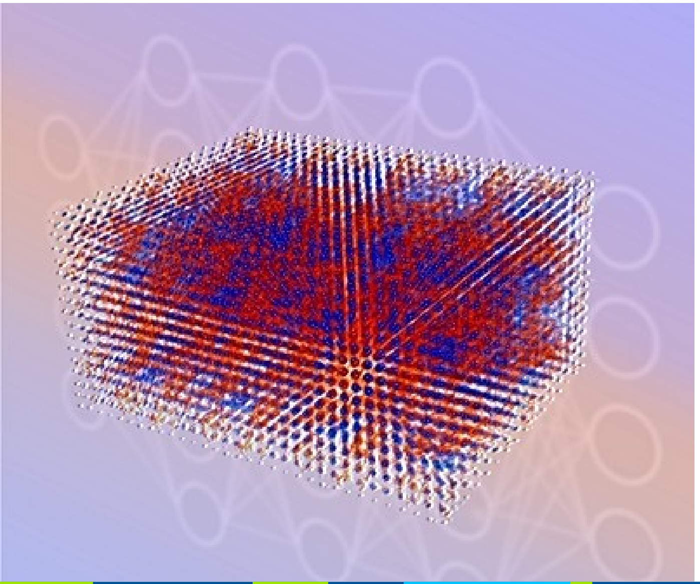
HiPACE++ → VisualPIC
Credit: M.Thévenet
& A. Ferran Pousa (DESY)



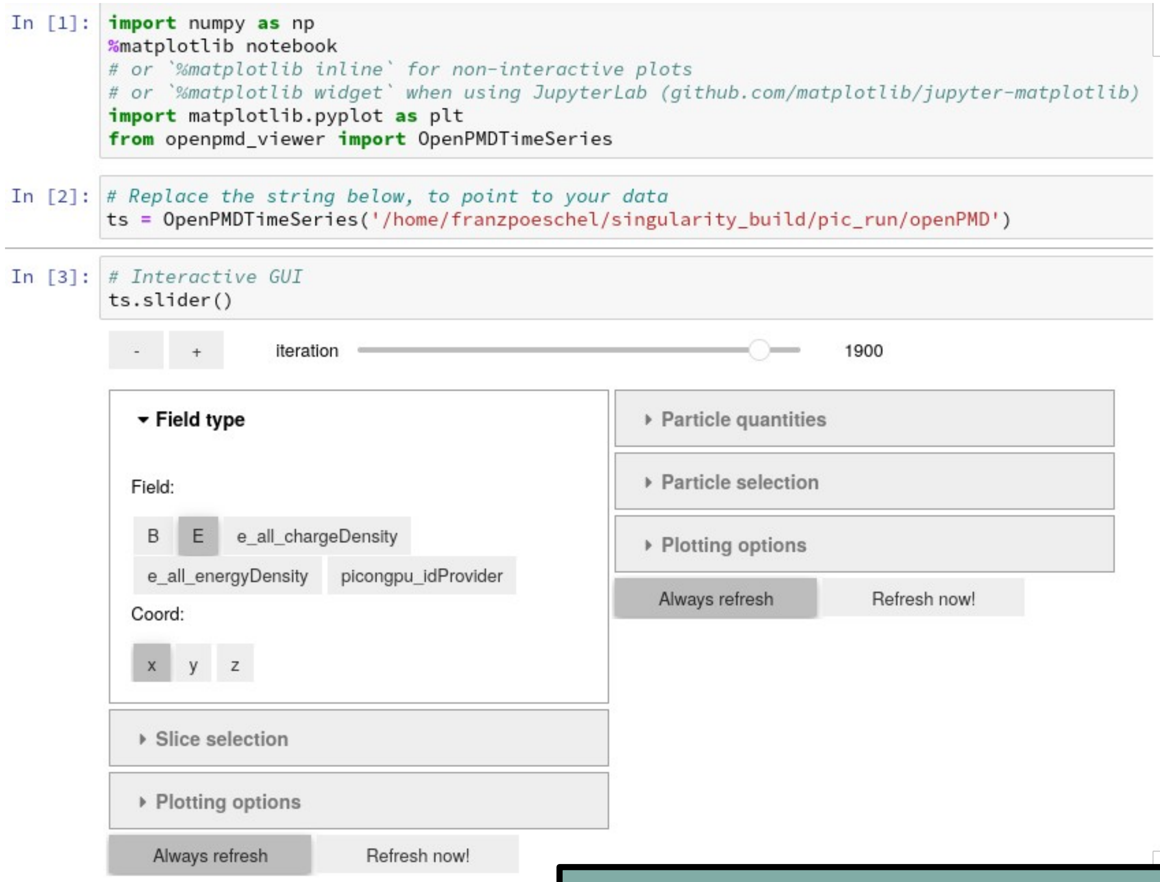


MALA → ParaView
Credit: A. Cangi (CASUS)

- **Wake-T** (DESY)
  fast particle-tracking code for plasma-based accelerators
  maintainer: A Ferran Pousa
- **HiPACE++** (DESY, LBNL)
  3D GPU-capable quasi-static PIC code for plasma accel.
  maintainers: M Thevenet, S Diederichs, A Huebl
- **Bmad** (Cornell)
  library for charged-particle dynamics simulations
  maintainers: D Sagan et al.
- **MALA** (CASUS, SNL)
  ML models that replace DFT calculations in materials science
  maintainers: Attila Cangi & Sivasankaran Rajamanickam
- and more…

see also: https://github.com/openPMD/openPMD-projects

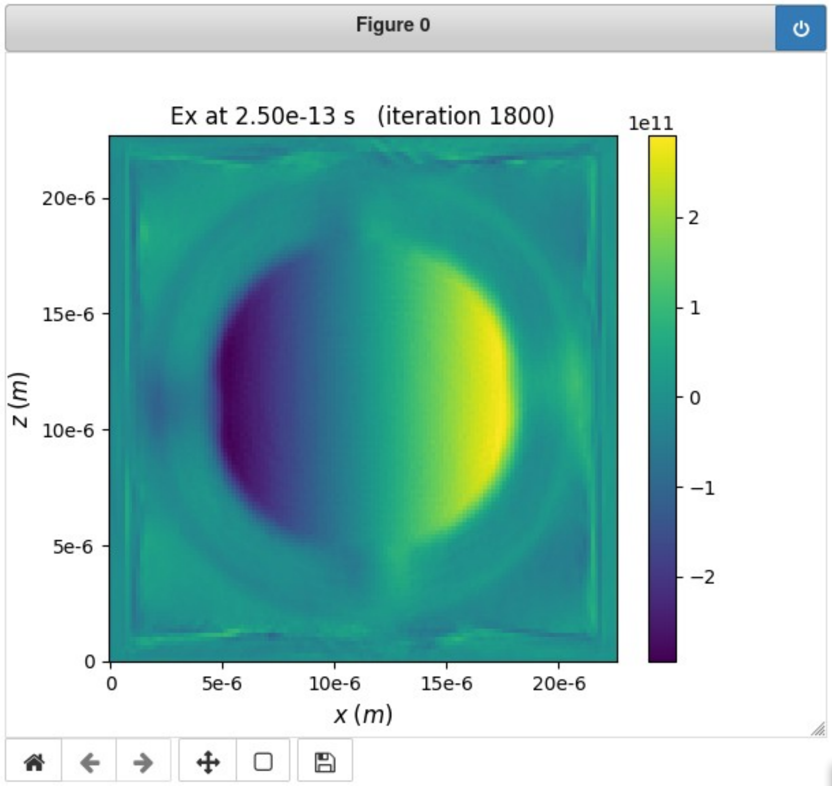
Analysis and Visualization



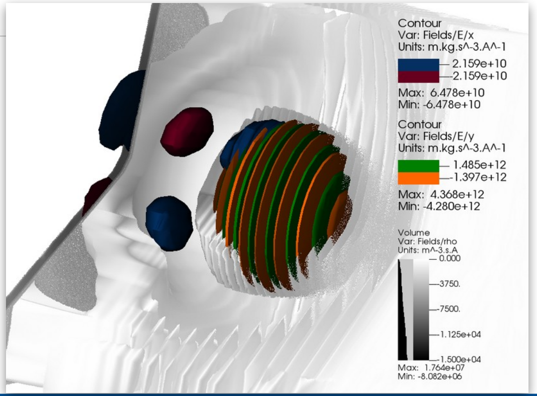
```
In [1]: import numpy as np
        %matplotlib notebook
        # or `%matplotlib inline` for non-interactive plots
        # or `%matplotlib widget` when using JupyterLab (github.com/matplotlib/jupyter-matplotlib)
        import matplotlib.pyplot as plt
        from openpmd_viewer import OpenPMDTimeSeries

In [2]: # Replace the string below, to point to your data
        ts = OpenPMDTimeSeries('/home/franzpoeschel/singularity_build/pic_run/openPMD')

In [3]: # Interactive GUI
        ts.slider()
```



openPMD/openPMD-viewer



Standardization of data

→ integration into modern scientific compute workflows

RAPIDS pandas openPMD DASK ParaView yt VisIt

Current status and Todo

Done:

- Added a Fortran module openPMD.F to bind to the C++ API via C
- Modified cp_output_handling.F module to support creation of openPMD files instead of Cube
- Challenges:
  - openPMD has an internal structure, hence one openPMD file corresponds to multiple Cube files
    → Need to distinguish callsites
  - Streaming support requires a workflow where IO handles stay open in the background
  - Representation for nested Iterations

To do:

- Actually write n-dimensional output
  (in realspace_grid_cube.F)
- Parallel output (best-case scenario: trivial)
- Input reading from openPMD
- Runtime configuration via input files
- Conditional compilation
  (openPMD as an optional dependency)
- Add openPMD output to modules other than src/qs_scf_post_gpw.F
  Should be simple once the main logic stands.
- Testing, tooling (e.g. conversion Cube ←→ openPMD)

Thomas Kühne/CASUS

- Sigma-RPA (Görling) implementation nearly done, benchmark tests currently ongoing
- MACE-potential meeting -> periodic RPA calculations (CP2K) needed to train networks
- HPC events:
  - NVIDIA GPU-event
  - Jülich recently
- (cusolvermp generalized eigenvalue solver)
- Caution for ELPA: make sure that you use
  - CPU: 2-stage solvers
  - GPU:1-stage solvers
  - see also https://manual.cp2k.org/trunk/CP2K_INPUT/FORCE_EVAL/PW_DFT/CONTROL.html and benchmark for your case!
- Announcement:
  - PostDoc position open in Stefan Grimme‘s group

„Traditional“ Diagonalization

$$\mathbf{K}\mathbf{c} = \mathbf{S}\mathbf{c}\epsilon$$

$$\boldsymbol{K}\,\mathbf{c} = \boldsymbol{U}^{\mathrm{T}}\boldsymbol{U}\,\boldsymbol{c}\,\epsilon$$

$$(\boldsymbol{U}^{\mathrm{T}})^{-1}\,\boldsymbol{K}\,\boldsymbol{U}^{-1}\,\boldsymbol{c}' = \boldsymbol{c}'\,\epsilon$$

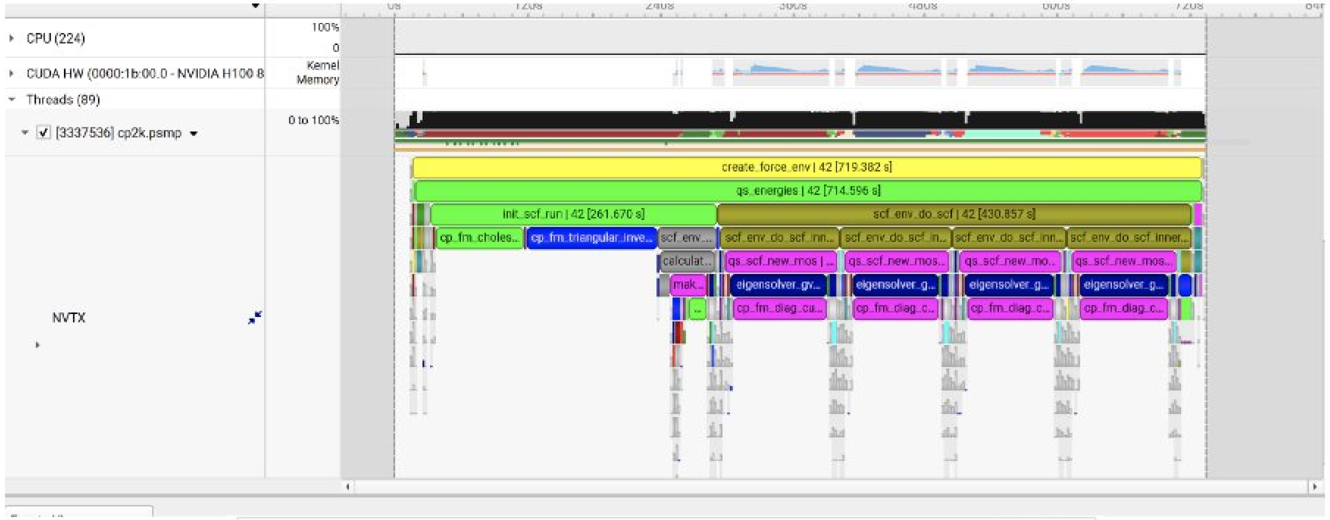
(`pdsygst`)

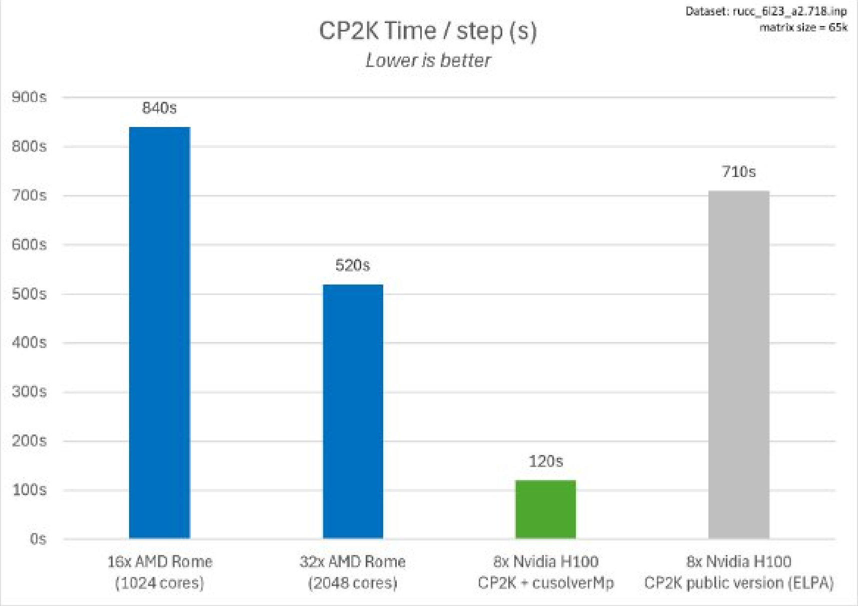
$$\boldsymbol{K}'\,\boldsymbol{c}' = \boldsymbol{c}'\,\epsilon$$

(`pdsyevx` or `pdsyevd`)

$$\begin{aligned} \mathbf{c} &= \mathbf{U}^{-1}\mathbf{c}' \quad \text{or} \\ \mathbf{c} &= \mathbf{S}^{-1/2}\mathbf{c}' \end{aligned}$$

„Traditional“ Diagonalization





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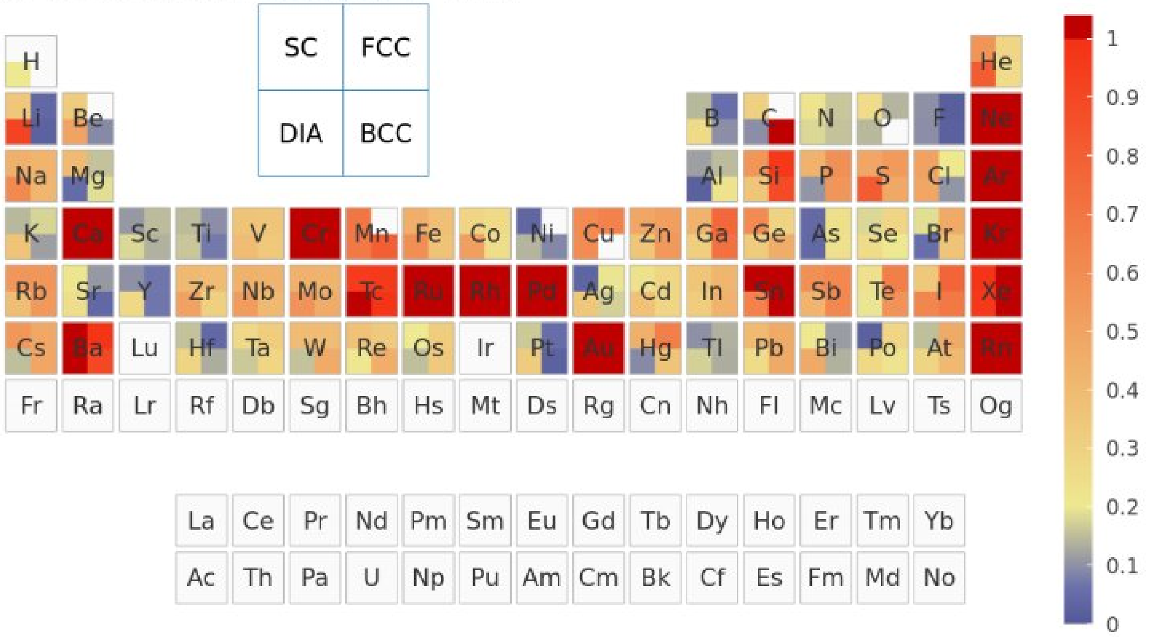
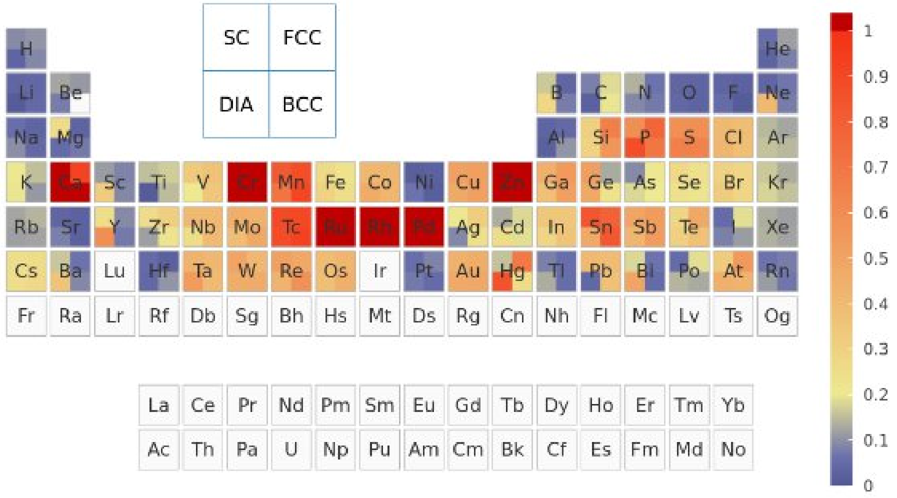
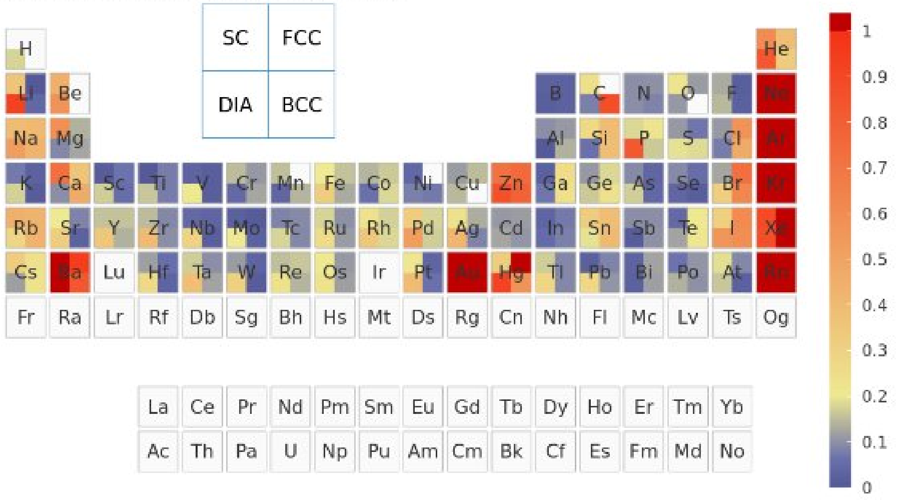
ε for CP2K-GTH-UZH vs. SIRIUS-FP-LAPW



ε for SIRIUS-GTH-UZH vs. SIRIUS-FP-LAPW

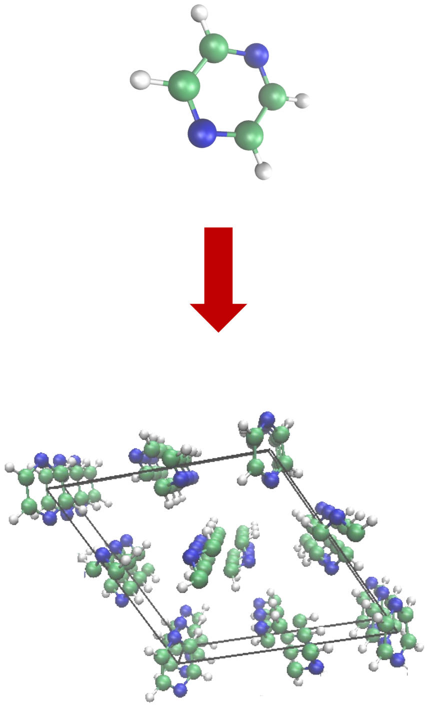


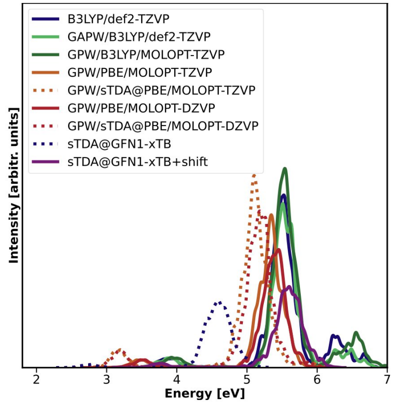
ε for CP2K-GTH-UZH vs. SIRIUS-GTH-UZH

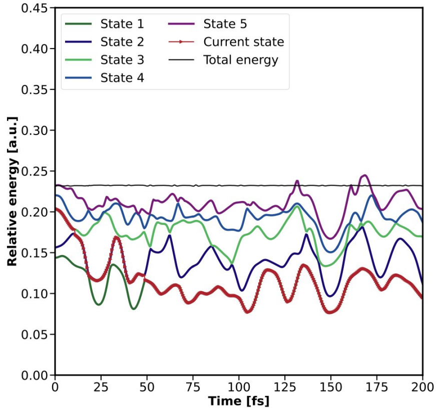


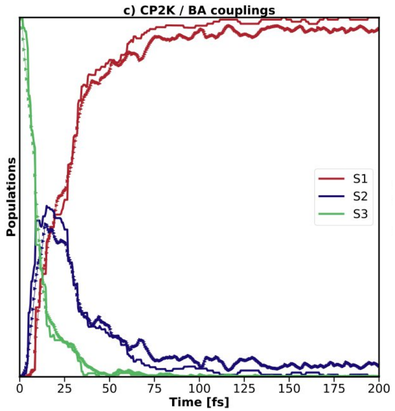
Ongoing developments in Kiel

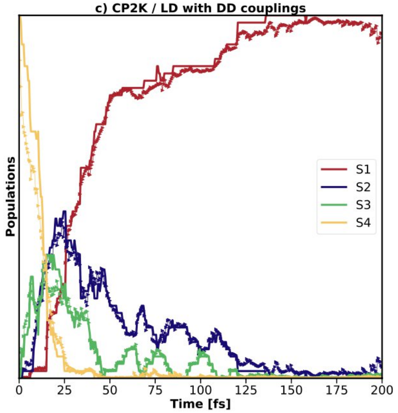
- **Non-adiabatic molecular dynamics** relying on semi-empirical or fast numerical time derivative couplings or local diabatization
- **Smeared occupation** for time-dependent density functional theory ansätze to capture static correlation (based on different distribution functions)
- **Simplified Bethe-Salpeter equation** and multipole expansions for GFN1-xTB (CRC proposal)

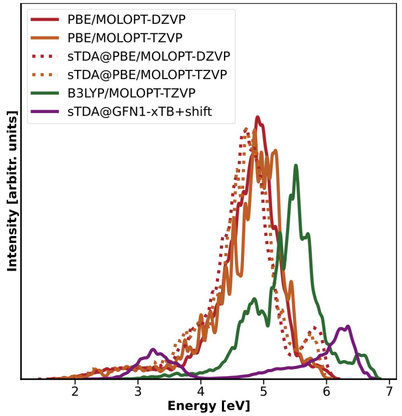


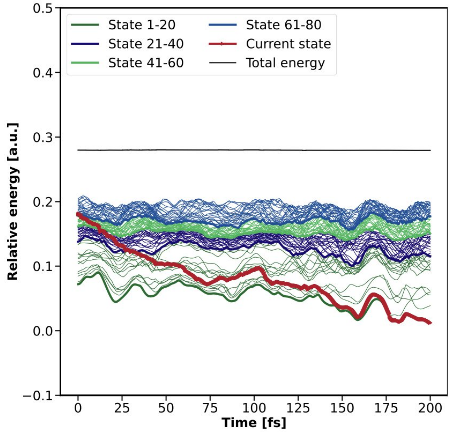


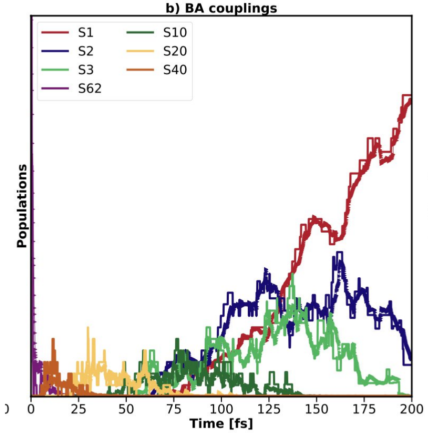


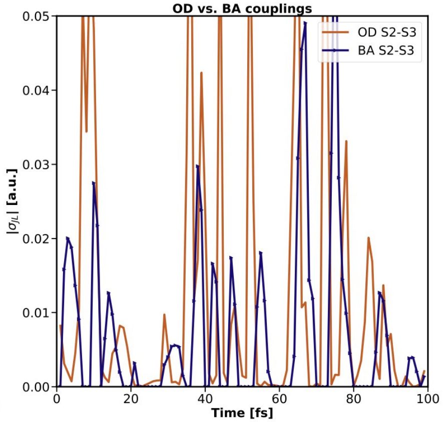












Current Issues in CP2K

- PR #4000: significant perf. overhead if F2K8+ compliant behaviour like copy/assignment (re-)allocation
  - Issue appeared with IFX but after fix, GNU had significant benefit too
  - Related to structures with allocatable components
- OpenMP workshare incorrect in almost all compiler (https://github.com/cp2k/dbcsr/issues/857#issuecomment-2511098676)

Next CP2K Release

- Schedule: Summer 2025
  - Makefile deprecation
  - CMake support

Planned Events in the Context of CP2K

- International Summer School on CP2K-GROMACS for Multiscale Atomistic Simulation
  - tentative date: 4 days in KW 40 (29.9. - 2.10.) at Uni-Paderborn (depends on availability of room)
  - tentative programs: lectures + hands-on exercises + posters from participants
  - tentative schedule:
    - day 1: GROMACS and MD Simulation
    - day 2: CP2K, Intro to QM/MM, CP2K/GROMACS QM/MM Simulation
    - day 3: IC-QM/MM and Post-DFT in CP2K
    - day 4: GROMACS on GPUs and MiMiC

Planned Events in the Context of CP2K

- next LUMI hackathon (Oslo): https://lumi-supercomputer.eu/events/lumi-hackathon-spring2025/
- next-to-next hackathon (CSCS): November
- Juelich Mimic Summer school: 1st week of June, CECAM+Psi-k https://www.cecam.org/workshop-details/multiscale-molecular-dynamics-with-mimic-optimizing-the-performance-on-modern-supercomputers-1397

Part 2: GPU Development in CP2K

1. Portable CUDA Concept (Ole Schütt)
2. Other GPU Programming Topics

Portable CUDA Concept (Ole Schütt)

- Use the subset of CUDA that's also supported by HIP.
- Use our offload API to switch between runtimes.
- Full code sharing between Nvidia and AMD.
- Partial code sharing with OpenCL / Intel.
- Partial code sharing with CPU.
- Simple, robust, and future proof.
- Successfully in use for grid, DBM, and pw.

Why doesn't anyone else advertise this? (speculations)

- It's boring. CUDA has been around since 2006.
- GPU manufacturers prefer solutions with vendor lock-in.
- Computing centers don't like to admit that GPUs require large rewrites.

Comments

- https://x-dev.pages.jsc.fz-juelich.de/models/
- Hipfly (header based translation) approach where one can keep their CUDA code and translate to HIP at compile time: https://github.com/amd/HPCTrainingExamples/tree/main/hipifly/vector_add
- Do concurrent: depends a lot on the compiler support

Other GPU Programming Topics (HansP)

- __OFFLOAD_UNIFIED_MEMORY

  PROs

  - Enables more GPU usage (finer granularity)?

  CONs

  - Less explicit/general compared to assuming descrete memory spaces
  - Unclear performance status wrt level of hardware support

  Optional

  - Asks to fold host and device pointers (code and data structures affected)
  - Currently, H2D and D2H are no-ops, only “host“-pointers are allocated

- How about GPU-CPU hybrid computations?
  - For example, DBM could use both CPU and GPU...

Comments

- Ongoing work for MI300A, grid code already ported to unified memory