openPMD

the Open Standard for Particle-Mesh Data

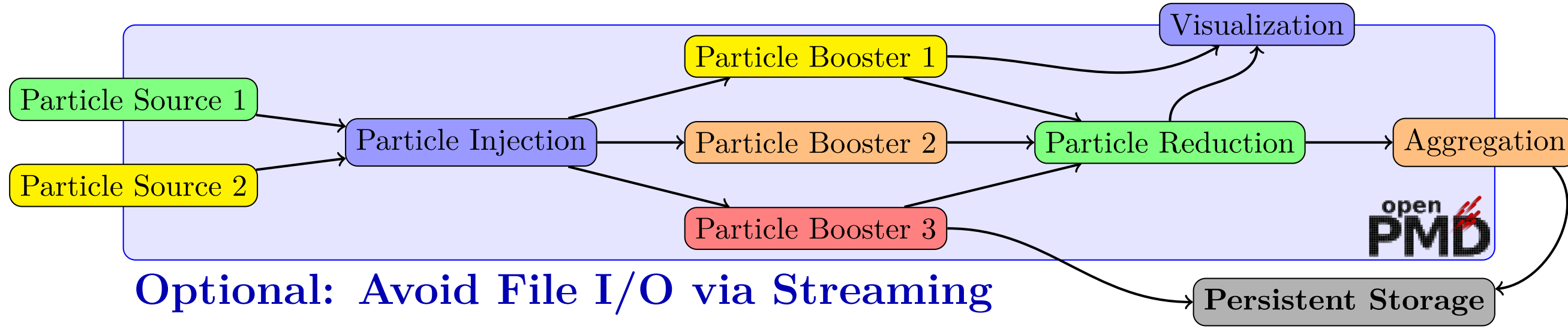**CASUS** — CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

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www.openPMD.org
github.com/openPMD

Heterogeneity through Standardized Data

Optional: Avoid File I/O via Streaming

Scientific compute workflows are complex:
- need to span different **time** and **length scales**
- particle accelerator modeling requires **multiple codes**, collaborating in a **data processing pipeline**
- **bridge heterogeneous models** by standardization of data

HELPMI – a project by the HMC

- explore a F.A.I.R. standard for laser-plasma *experiments*
- project from April 2023 to April 2025

openPMD's role
- background: LPA *simulations*
- HELPMI aims to close the gap between openPMD and NeXus
- aim for interoperability between openPMD + HELPMI + NeXus

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HI JENA Helmholtz-Institut Jena · HZDR HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF · CASUS CENTER FOR ADVANCED SYSTEMS UNDERSTANDING · GSI
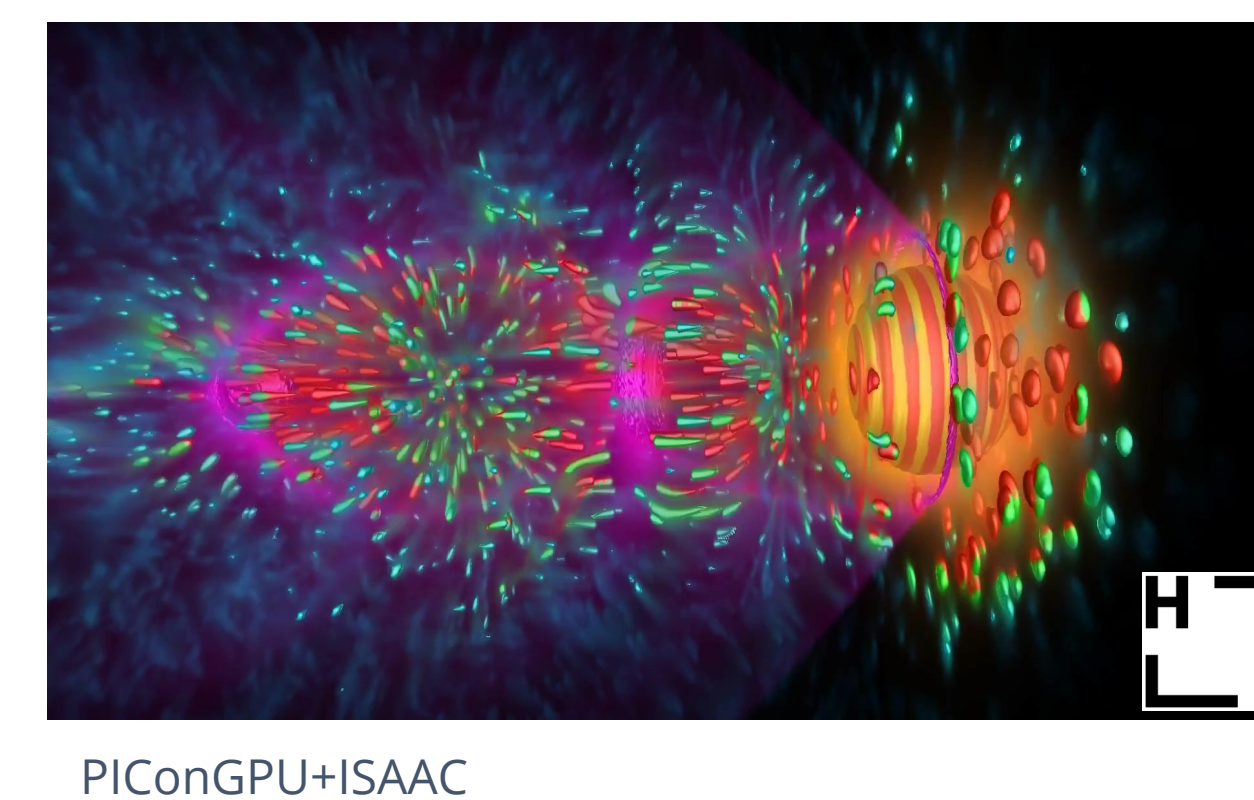
openPMD Ecosystem

File markup and definition:
openPMD standard (1.0.0, 1.0.1, 1.1.0)

Ref. Implementation and Bindings:
openPMD-api[LBNL, CASUS, HZDR]:

- express **data description** in a C++/Python/(dev) Julia API **backend-agnostically**, **configuring the I/O backend at runtime**
- still use full functionality of underlying I/O libraries (**compression, aggregation, staging, strides, ...**) and their native tooling

HiPACE++ → openPMD → VisualPIC
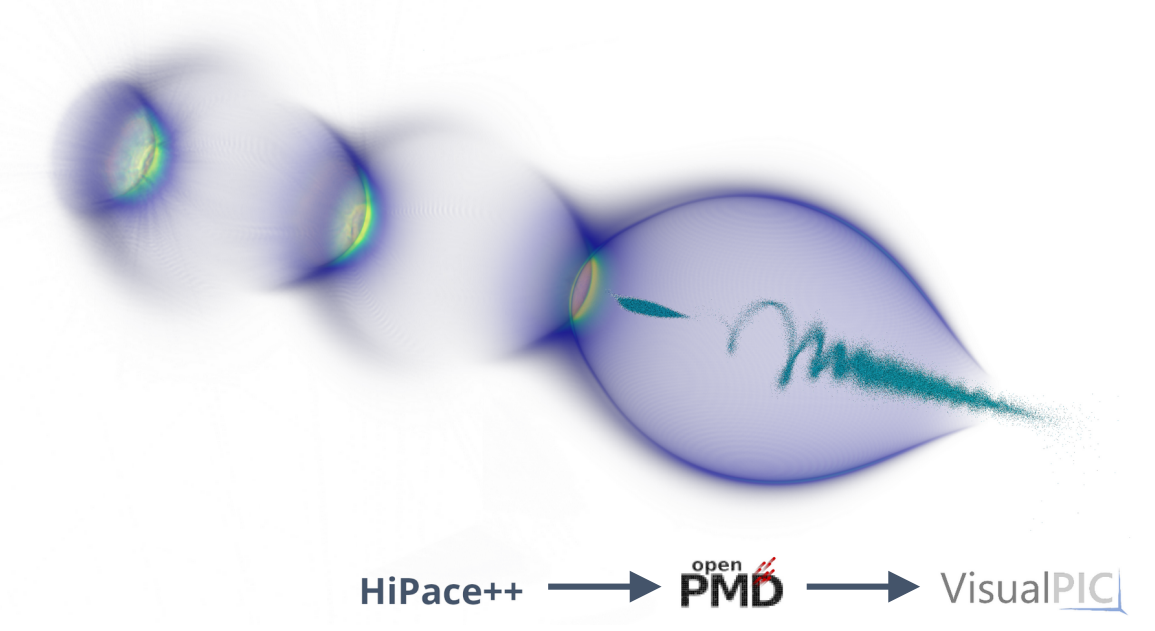
- open development & tests: github.com/openPMD/openPMD-api
- available in common package managers and deployed on HPC systems

Python-Pip · Conda · Homebrew · Spack · CMake · E4S + HPC modules


PIConGPU+ISAAC

Open Simulations with openPMD:

Examples: PIConGPU[HZDR], HiPACE++[DESY, LBNL], MALA[CASUS], BMAD[Cornell], Wake-T[DESY], SimEx Platform[EUCALL, European XFEL], FBPIC[LBNL, CFEL Hamburg University], WarpX[LBNL, DESY], ...

Data Processing and Visualization:
openPMD-viewer, VisIt, pyDive, postpic, yt project, ParaView, VisualPIC

Native tooling: HDF Compass, bpls
Integration into: Pandas, DASK, RAPIDS
file validators[HZDR, LBNL]

Full list: github.com/openPMD/openPMD-projects

Hierarchical organization of openPMD data

- **meta-standard:** truly self-describe data
- **open-access:** unified description
- **workflows:** high-level integrations
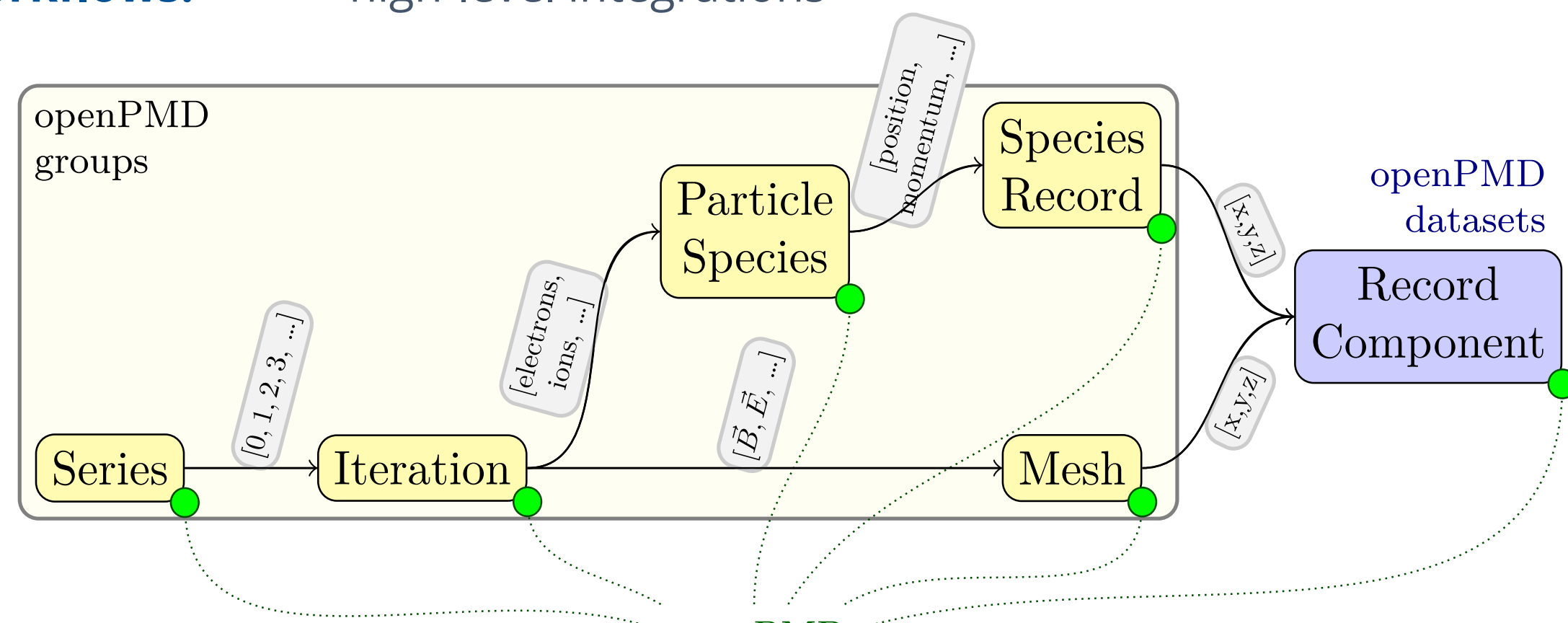
- particle and mesh based data
- data format agnostic
- frictionless data exchange

Findable: Standardized metadata to identify the data producer

```
string   /author          attr  = "franz"
string   /software        attr  = "PIConGPU"
string   /softwareVersion attr  = "0.5.0-dev"
```

**Accessible:** Open standard, implementable in various formats

ADIOS · The HDF Group

*currently implemented, but not limited to

Interoperable:
Data exchange spans applications, platforms and teams

Reusable:
Rich and standardized description for physical quantities

Scientific workflows need to bridge various applications and algorithms, ideally both **automatically-** und **human-readable**.

openPMD defines **scientific self-description**, usable in common storage/transport formats such as HDF5, ADIOS, JSON.
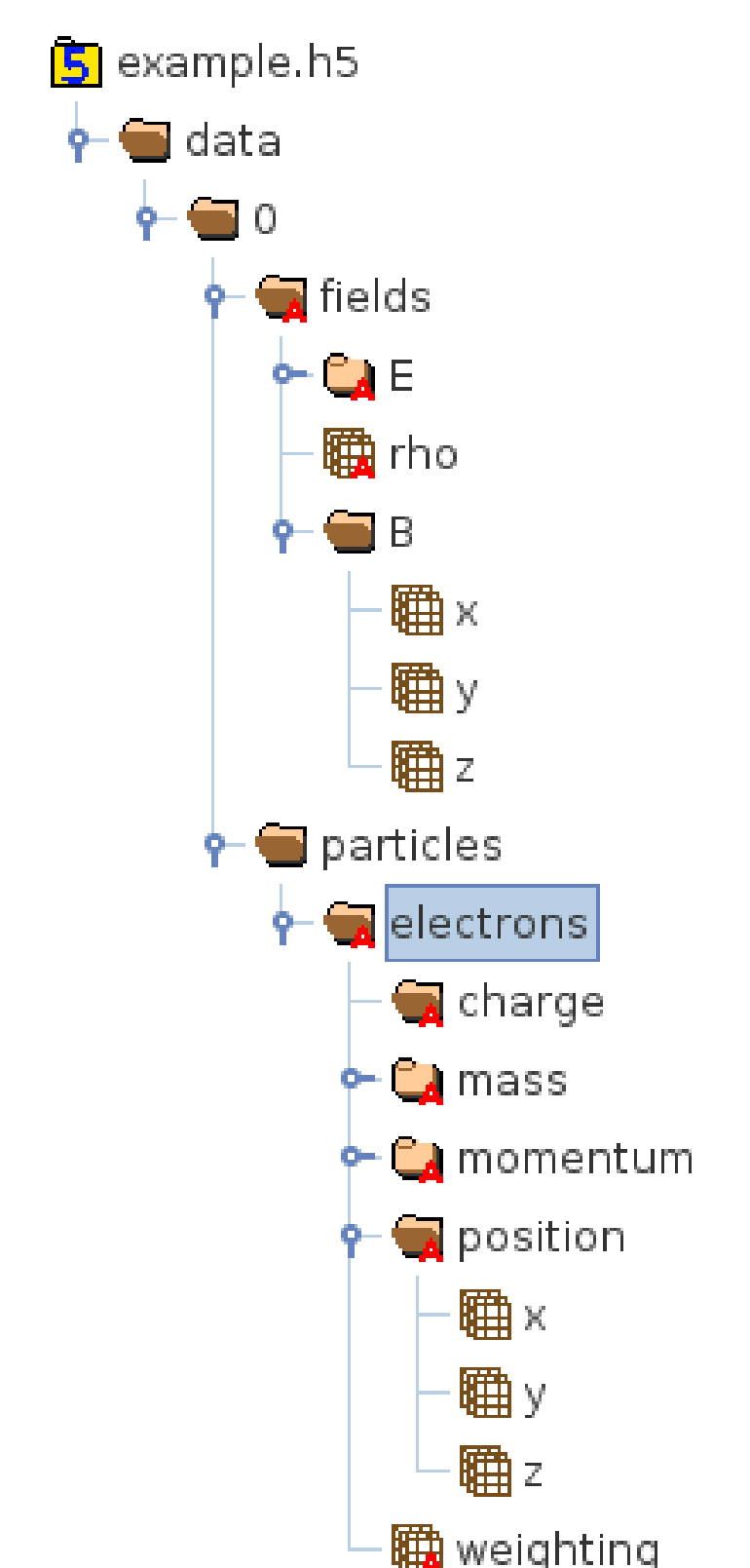
Axel Huebl et al. "openPMD: A meta data standard for particle and mesh based data". 2015. doi: 10.5281/zenodo.591699. url: https://openPMD.org

Compute Performance Outpaces Storage Performance

	Titan	Summit	Frontier
Peak Performance:	27 Pflop/s	200 Pflop/s	1.6 Eflop/s
FS Throughput:	1 TiByte/s	2.5 TiByte/s	5~10 TiByte/s
FS Capacity:	27 PiByte	250 PiByte	500~1000 PiByte

Franz Poeschel et al. "Transitioning from file-based HPC workflows to streaming data pipelines with openPMD and ADIOS2". 2022. doi: 10.1007/978-3-030-96498-6_6.

Break through Filesystem Bandwidth with Streaming: >2.5TiByte/s

PFS bandwidth limit

IO Gap

ADIOS PIConGPU

- stream throughput
- file throughput (1 writer per node)
- file throughput (6 writers per node)
- extrapolated ideal parallel scaling

total perceived throughput [GiByte · s^{-1}]
number of nodes

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