Open Science with openPMD

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the **meta-data standard**

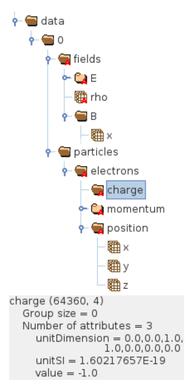
- **p**article and **m**esh based **d**ata
- **data format agnostic**
- **frictionless data exchange**

www.openPMD.org

github.com/openPMD

Self-Description is a Challenge

Scientific workflows need to *bridge* various applications and algorithms, ideally both **automatically**- and **human-readable**.
Our *glue*, using a **hierarchical file format** such as HDF5, ADIOS BP, XML, JSON, is not automatically **scientifically self-describing**.



minimal set/kernel of meta information

- **meta-standard**: truly self-describe data (sinks & sources)
- **open-access**: unified description (creation → publishing)
- **workflows**: high-level integrations (apps, visualization markups)

Key Concepts by Example

electric field $\vec{E}(\vec{r})$: ← **record**

/ ... / meshes / E / x, y, z ← **component**

.unitSI, .unitDimension,

.geometry, .time, ... ← **attribute**

electron charge Q_i: ← **group**

/ ... / particles / electrons / Q_i

.unitSI, ...

A strict grouping but flexible naming of **records** allows easy parsing and traversal.

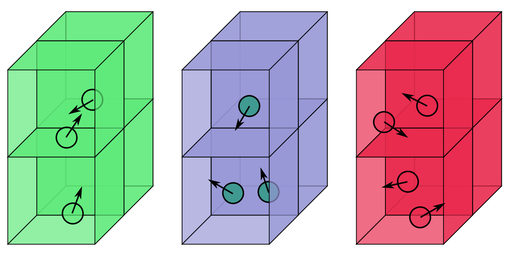
Heavy data is guaranteed to stay contiguous for performant I/O. Light-weight annotations are buffered and read/written at once.

Example for the structure of an openPMD annotated data set. From a user-point of view, **records** are the central objects to be described.

Exascale Computing Needs Multi-PByte Scalable, Documented Data

User-space expressible:

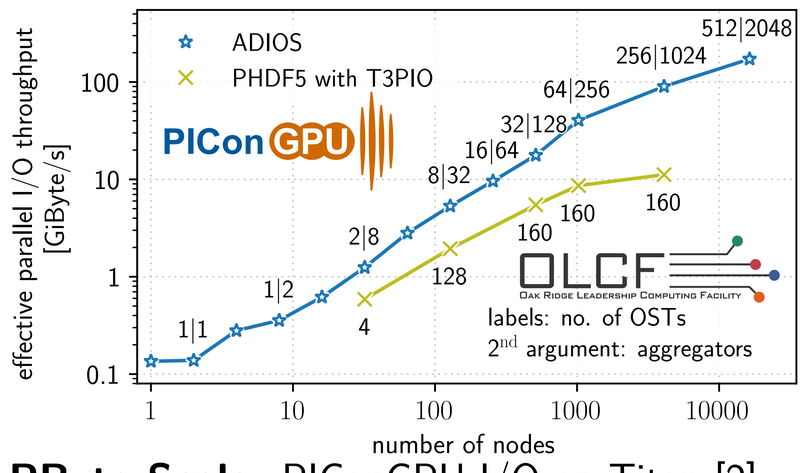
- constant record components
- domain patches



Still full functionality of **underlying I/O libraries**:

- ➢ portability
- ➢ internal / external links
- ➢ strides, aggregations, multi-file
- ➢ compression [2], staging [3,4]

Integrated and long **staged I/O pipelines** will be essential for I/O in **Exascale HPC**. Meta-data must easily *propagate* and *be usable* at any stage and time.



PByte-Scale: PIConGPU I/O on Titan [2]

Open Science Attracts Collaboration

source: open, contributable
review: open issues/updates
methodology: documented workflows
education: resources & integrations
data: versioned, self-describing

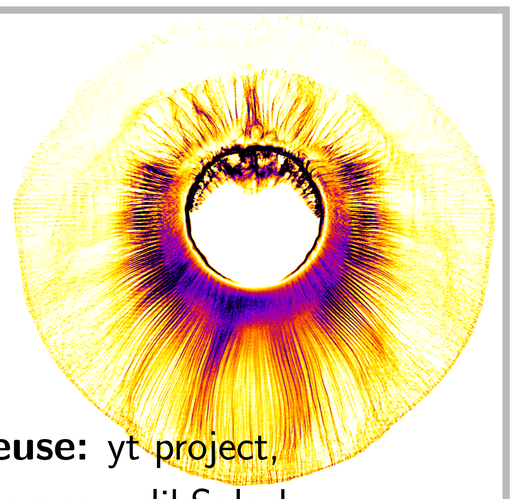
→ **reproducibility**, **quality**, **sustainability**, **exchange**, **after-use**

Open Simulations:

PIConGPU[HZDR], ParaTAXIS[HZDR], openFPM[MPI-CBG], Warp[LBNL, LLNL], FBPIC[LBNL, DESY], SIMEX[EUCALL]

Open Post-Processing:

openPMD-viewer + **contribute & reuse:** yt project, VisIt, postpic, pyDive, XDMF, HDF Compass, libSplash, ...



[1] A. Huebl et al. *openPMD 1.0.0: A meta data standard for particle and mesh based data*, technical specification (CC-BY 4.0), November 2015, DOI:10.5281/zenodo.33624 [2] A. Huebl et al. *On the Scalability of Data Reduction Techniques in Current and Upcoming HPC Systems from an Application Perspective*, ISC 2017, arXiv:1706.00522 [3] H. Abbasi et al. *Datastager: scalable data staging services for petascale applications*, Cluster Computing 13(3), DOI:10.1007/s10586-010-0135-6 [4] C. Docan et al. *DataSpaces: An interaction and coordination framework or coupled simulation workflows*, HPDC 2010, DOI:10.1007/s10586-011-0162-y

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