openPMD

CASUS
CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

www.casus.science

Plasma-PEPSC Workshop
23 October 2024

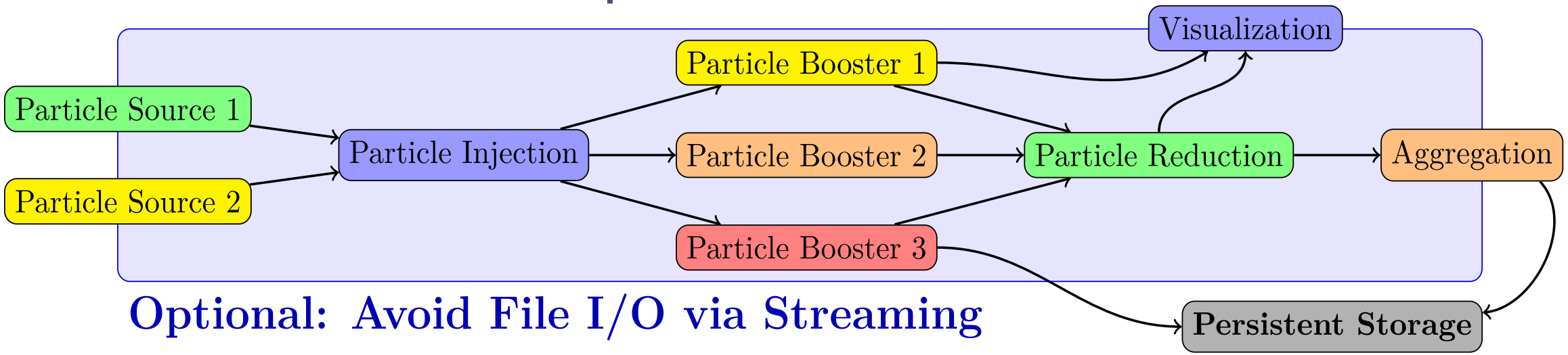
The Open Standard for Particle-Mesh Data

HZDR HELMHOLTZ ZENTRUM DRESDEN ROSSENDORF
TECHNISCHE UNIVERSITÄT DRESDEN
CBG Max Planck Institute of Molecular Cell Biology and Genetics
UFZ HELMHOLTZ Centre for Environmental Research
Uniwersytet Wrocławski

SPONSORED BY THE
Federal Ministry of Education and Research
STAATSMINISTERIUM FÜR WISSENSCHAFT KULTUR UND TOURISMUS
Freistaat SACHSEN

Heterogeneity through Standardized Data

Scientific workflows are complex:



Optional: Avoid File I/O via Streaming

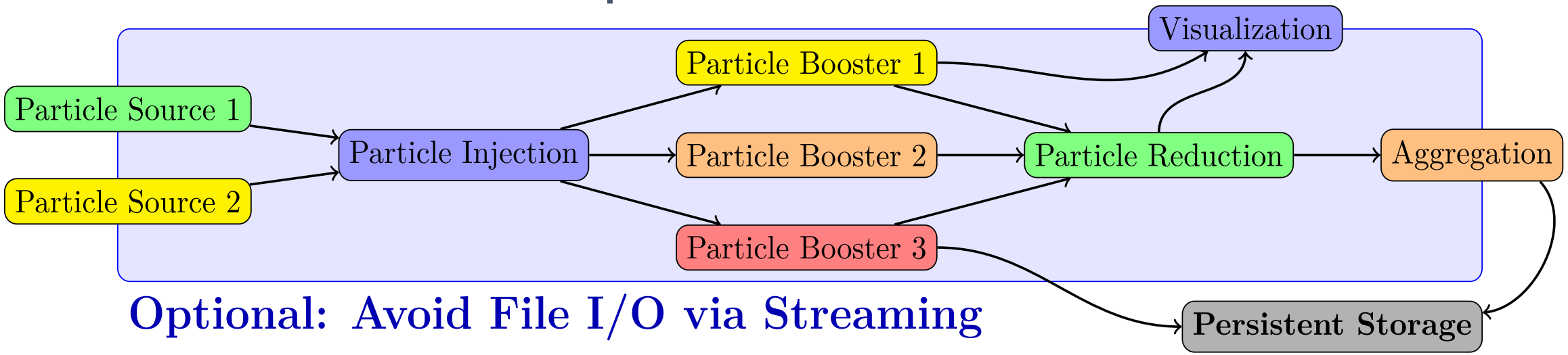
- need to span different **time** and **length scales**
- scientific modeling requires **multiple codes**, collaborating in a **data processing pipeline**
- **bridge heterogeneous models** by standardization of data

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

Franz Poeschel et al. “Transitioning from file-based HPC workflows to streaming data pipelines with openPMD and ADIOS2“. 2021. doi:10.1007/978-3-030-96498-6_6

Heterogeneity through Standardized Data

Scientific workflows are complex:



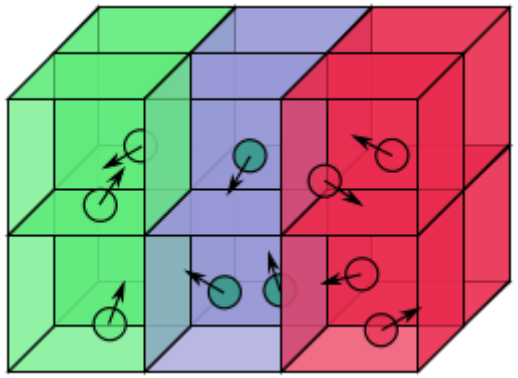
Optional: Avoid File I/O via Streaming

→ openPMD standard for **p**article-**m**esh **d**ata as communication layer

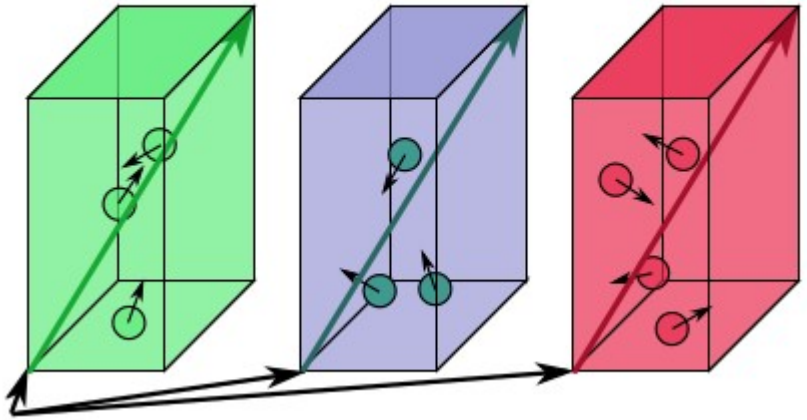
Axel Huebl et al. "openPMD: A meta data standard for particle and mesh based data". 2015. doi: 10.5281/zenodo.591699. url: https://openPMD.org

Franz Poeschel et al. "Transitioning from file-based HPC workflows to streaming data pipelines with openPMD and ADIOS2". 2021. doi:10.1007/978-3-030-96498-6_6

What is particle-mesh data?



[0:3] particles [3:6] particles [6:10] particles



Mesh

n-dimensional space,
divided into discrete cells

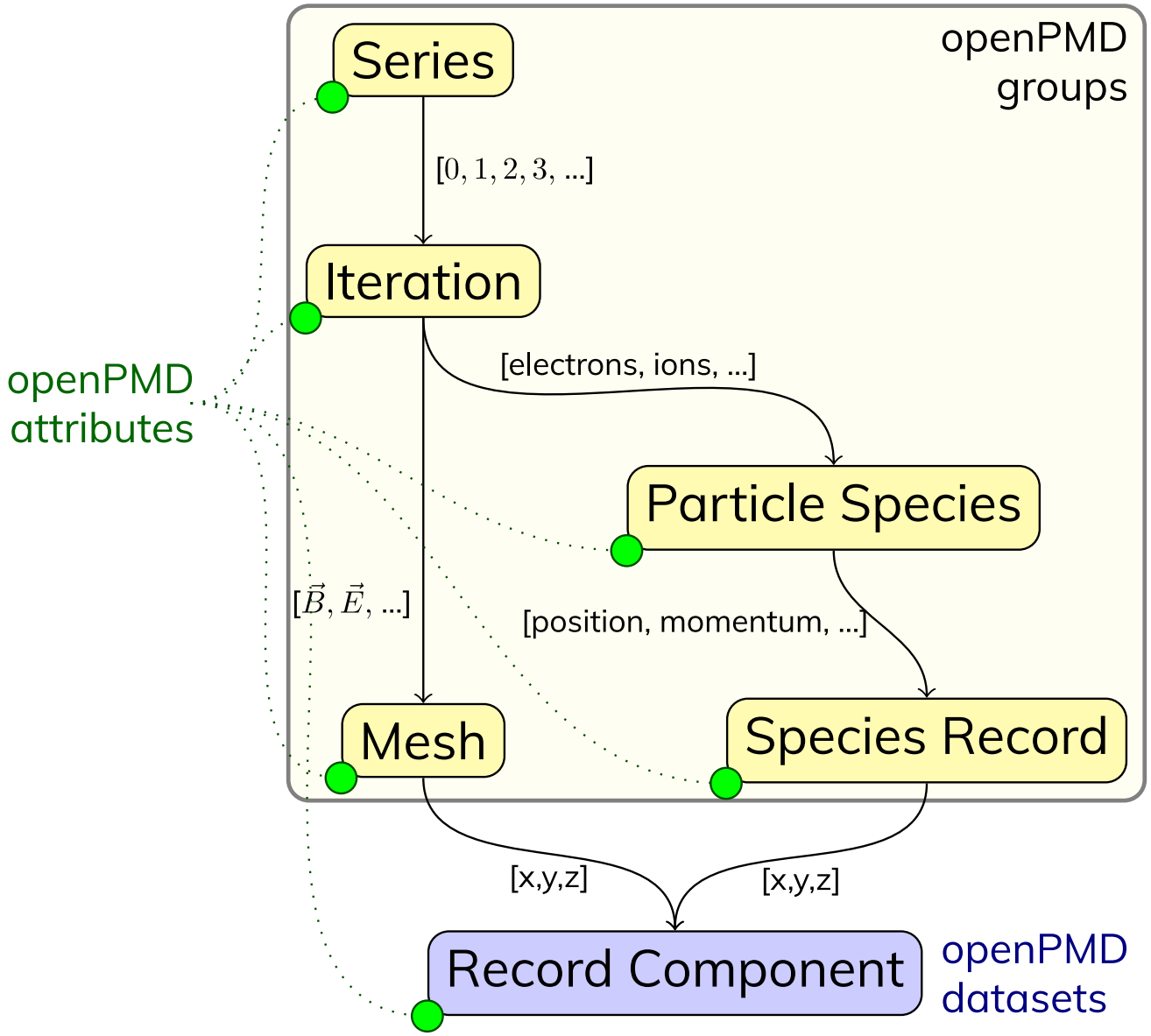
- e.g. temperature:
  store a scalar number per cell
- e.g. electrical fields:
  store a 3D vector per cell

Particles

A list of discrete objects,
located on the mesh

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

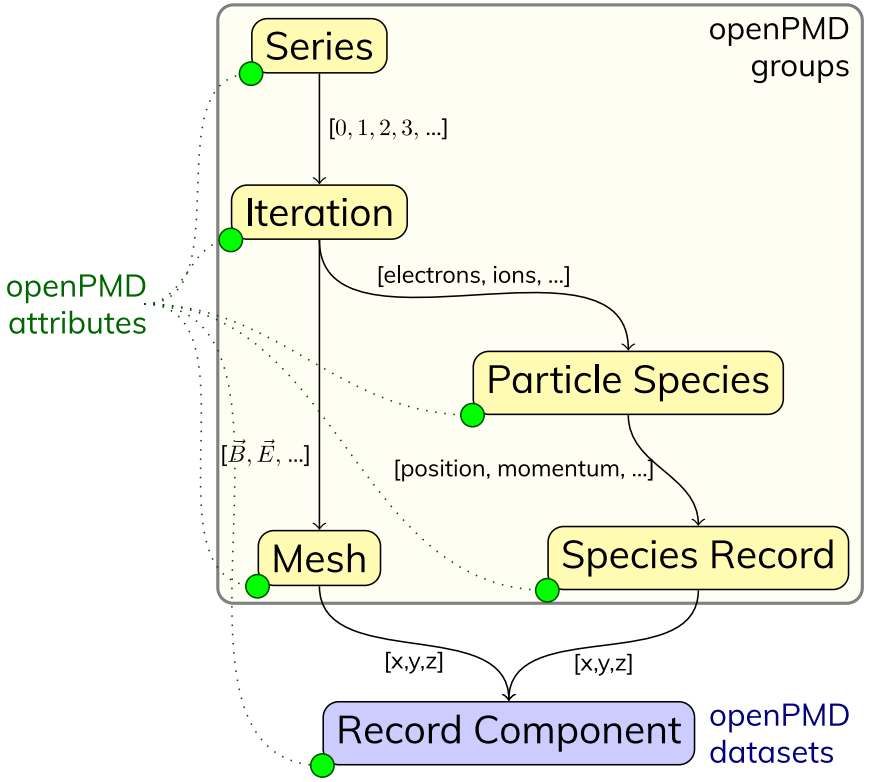
openPMD hierarchy



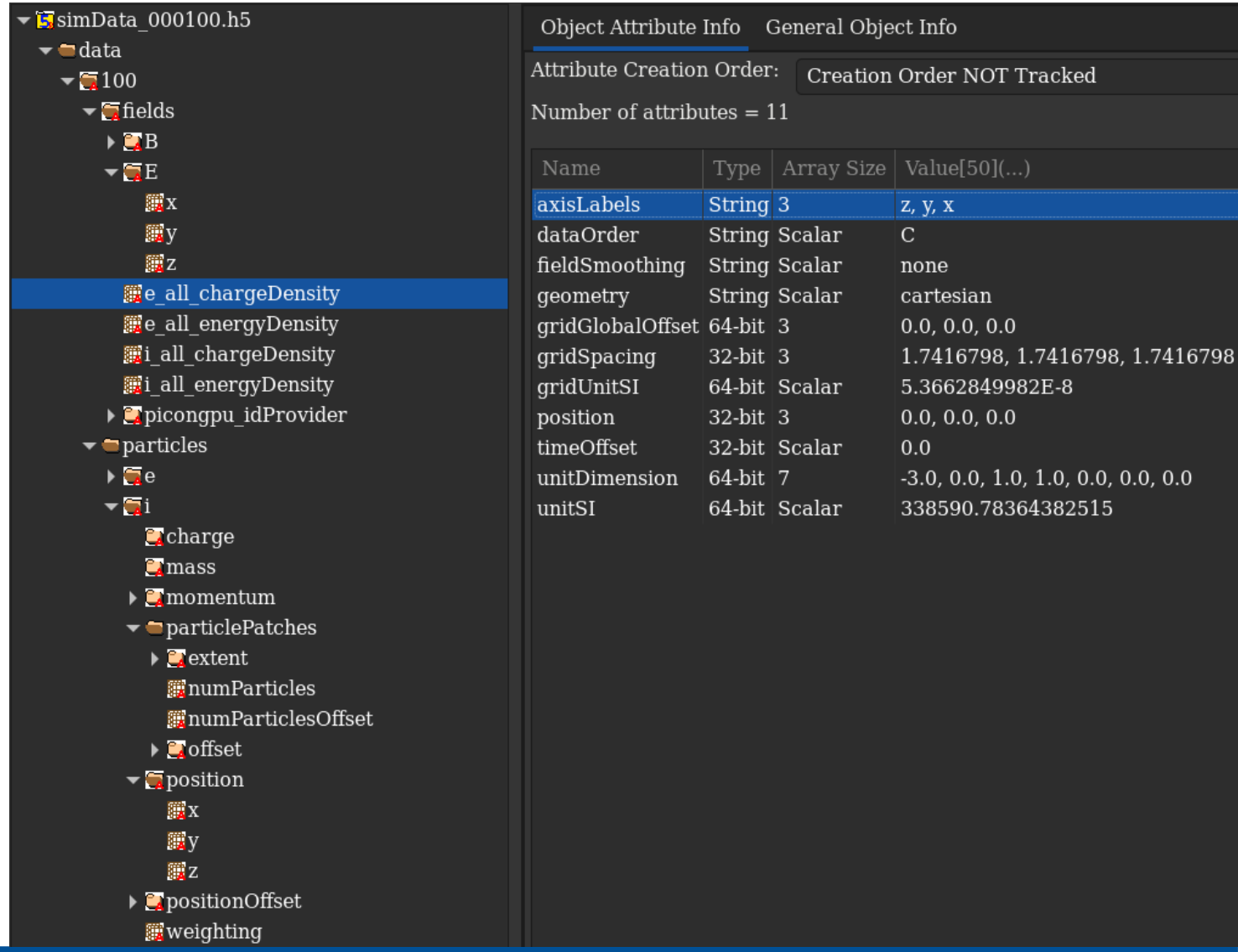
- **Structure** for series & snapshots encoded as either:
  - **files** (one file per iteration)
  - **groups** (reuse files)
  - **variables** (reuse files & variables in ADIOS2)

- 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



Example dataset: ADIOS2 backend

CASUS
CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

```
float     /data/50/fields/E/x                          {128, 128, 128}
float     /data/50/fields/E/y                          {128, 128, 128}
float     /data/50/fields/E/z                          {128, 128, 128}
float     /data/50/particles/e/position/x              {50053105}
float     /data/50/particles/e/position/y              {50053105}
float     /data/50/particles/e/position/z              {50053105}
int32_t   /data/50/particles/e/positionOffset/x        {50053105}
int32_t   /data/50/particles/e/positionOffset/y        {50053105}
int32_t   /data/50/particles/e/positionOffset/z        {50053105}
```

Hierarchical data organization

***n*-dim. datasets for heavyweight data**

```
string    /data/50/fields/E/axisLabels                 attr   = {"z", "y", "x"}
string    /data/50/fields/E/dataOrder                  attr   = "C"
string    /data/50/fields/E/fieldSmoothing             attr   = "none"
string    /data/50/fields/E/geometry                   attr   = "cartesian"
double    /data/50/fields/E/gridGlobalOffset           attr   = {0, 0, 0}
float     /data/50/fields/E/gridSpacing                attr   = {1.74168, 1.74168, 1.74168}
double    /data/50/fields/E/gridUnitSI                 attr   = 5.36628e-08
float     /data/50/fields/E/timeOffset                 attr   = 0
double    /data/50/fields/E/unitDimension              attr   = {1, 1, -3, -1, 0, 0, 0}
float     /data/50/fields/E/x/position                 attr   = {0.5, 0, 0}
double    /data/50/fields/E/x/unitSI                   attr   = 9.5224e+12
float     /data/50/fields/E/y/position                 attr   = {0, 0.5, 0}
double    /data/50/fields/E/y/unitSI                   attr   = 9.5224e+12
float     /data/50/fields/E/z/position                 attr   = {0, 0, 0.5}
double    /data/50/fields/E/z/unitSI                   attr   = 9.5224e+12
```

Attributes for self-description

Example dataset: JSON/TOML backend


```
{
  "attributes": {
    "basePath": "/data/%T/",
    "date": "2023-10-11 09:57:53 +0200",
    "iterationEncoding": "fileBased",
    "iterationFormat": "simData_%06T",
    "meshesPath": "fields/",
    "openPMD": "1.1.0",
    "openPMDextension": 0,
    "particlesPath": "particles/",
    "picongpuIOVersionMajor": 2,
    "picongpuIOVersionMinor": 0,
    "software": "PIConGPU",
    "softwareVersion": "0.7.0-dev"
  },
  "data": {
    "100": {
      "attributes": {
        "cell_depth": 4.252342224121094,
        "cell_height": 1.0630855560302734,
        "cell_width": 4.252342224121094,
        "dt": 1,
        "eps0": 169.19711303710938,
        "many": "more"
      },
      .....
```

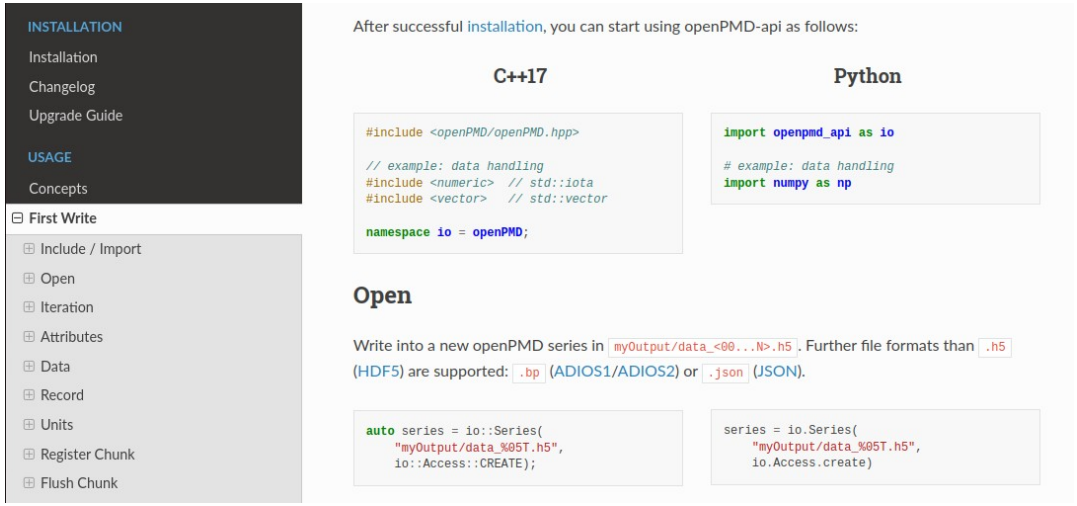
```
.....
"fields": {
  "e_all_energyDensity": {
    "attributes": {
      "axisLabels": [ "z", "y", "x" ],
      "geometry": "cartesian",
      "gridGlobalOffset": [ 0, 0, 0 ],
      "gridSpacing": [ 4.25, 1.06, 4.25 ],
      "gridUnitSI": 4.1671151662e-08,
      "position": [ 0, 0, 0 ],
      "timeOffset": 0,
      "unitDimension": [ -1, 1, -2, 0, 0, 0, 0 ],
      "unitSI": 7869098408118.734
    },
    "datatype": "FLOAT",
    "data": [
      [
        [
          "multidimensional dataset here"
        ]
      ]
    ]
  }
}
}
}
}
```

- Part of the package: No need to install 3rd-party dependencies
- Useful for debugging and prototyping
- Limited parallel support
- Courtesy to Nils Lohmann‘s JSON library for C++
- With recent release: Convert output to TOML Idea: openPMD formatted configuration files

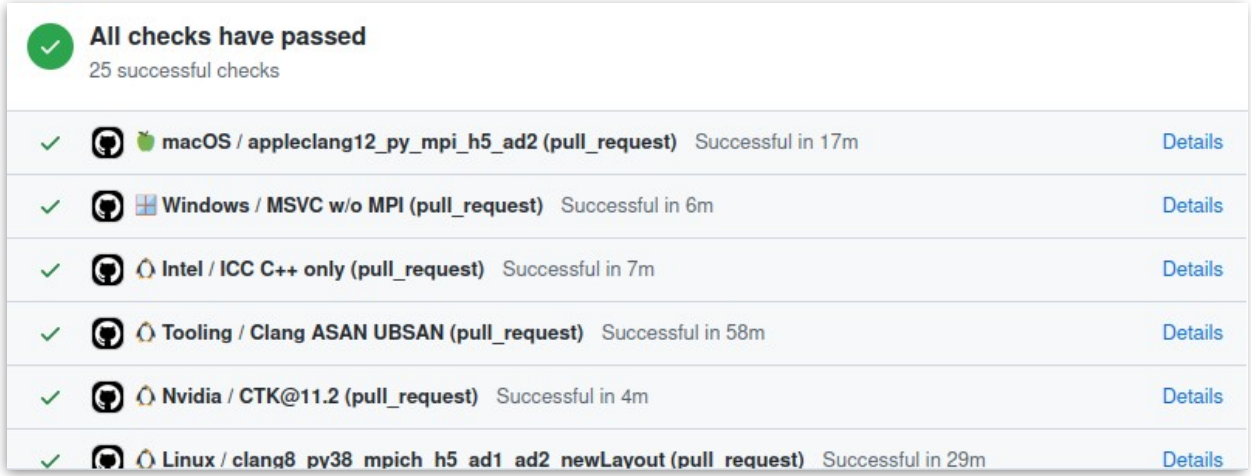
Reference Implementation in C++ & Bindings: Python and Julia

CASUS
CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

Online Documentation: openpmd-api.readthedocs.io



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



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
```

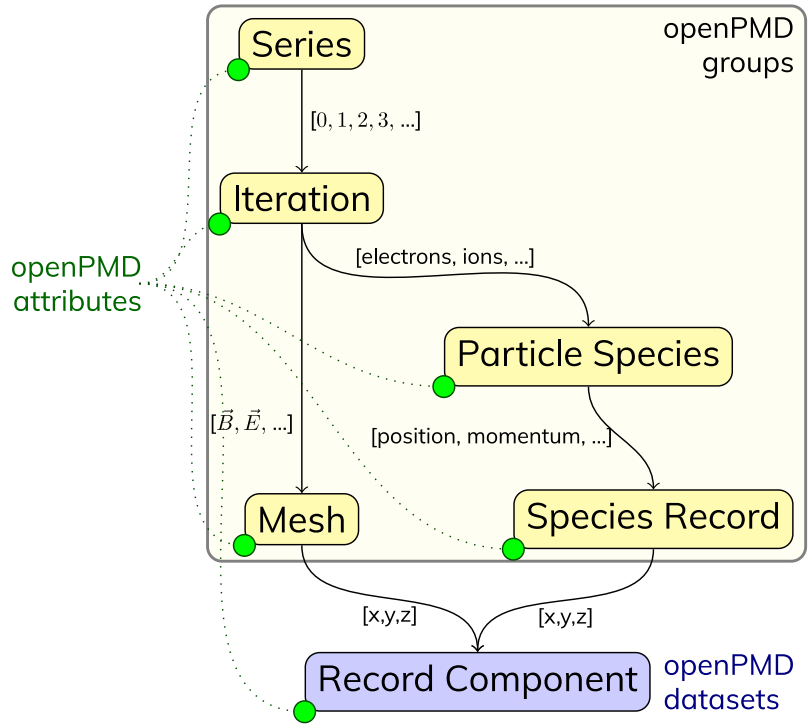

```
module load openpmd-api
```

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

Hands-On:

openPMD-api:

basic object model



Module environment at `/project/project_465001310/workshop_software/env.sh`

Materials at `https://github.com/alpaka-group/alpaka-workshop-slides/tree/oct2024_workshop`

Read the `TODO` comments inside `src/openPMDOutput.hpp`:

Unit System

unitDimension

automated description of physical dimension

only powers of base dimensions

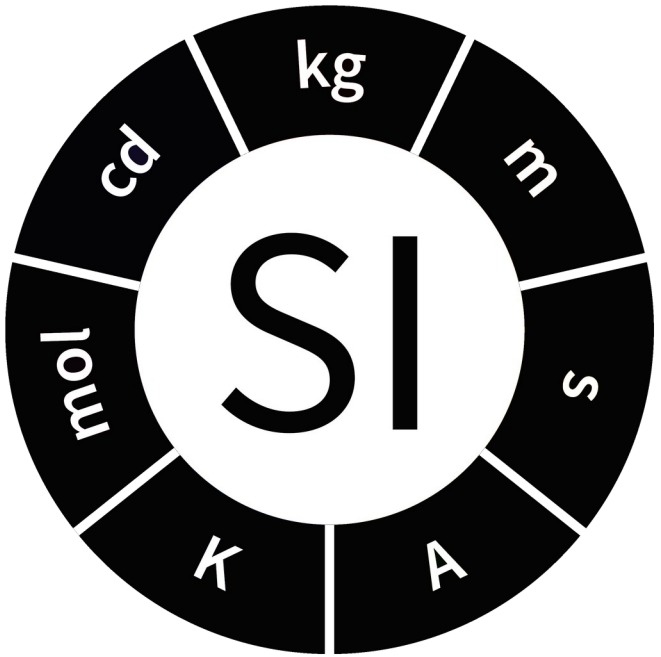
length **L**, mass **M**, time **T**, electric current **I**,
thermodynamic temperature **theta**,
amount of substance **N**, luminous intensity **J**

Magnetic field: $[B] = M / (I * T^2)$

→ (0, 1, -2, -1, 0, 0, 0)

unitSI (recommended)

relation to an absolute unit system



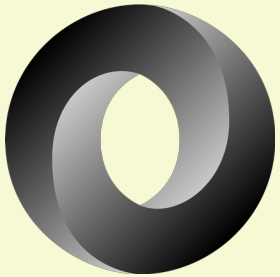
Wikimedia Commons

openPMD – a FAIR standard

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



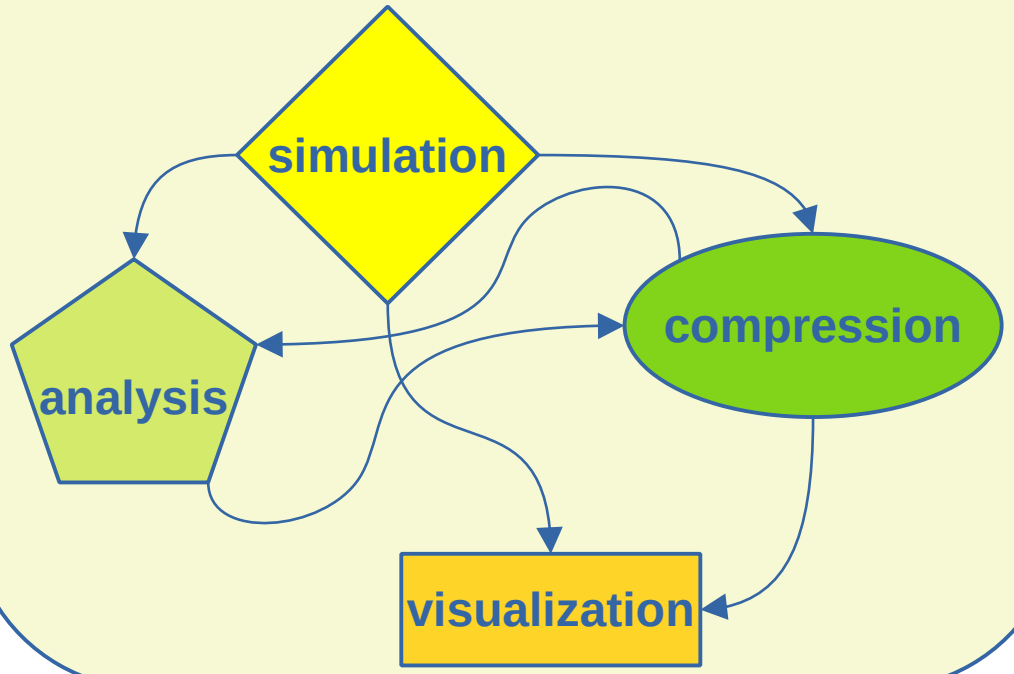
*currently implemented, but not limited to

"The FAIR Guiding Principles for scientific data management and stewardship" (Mark D. Wilkinson et al.)

openPMD – a FAIR standard

Interoperable:

Data exchange spans applications, platforms and teams



Reusable:

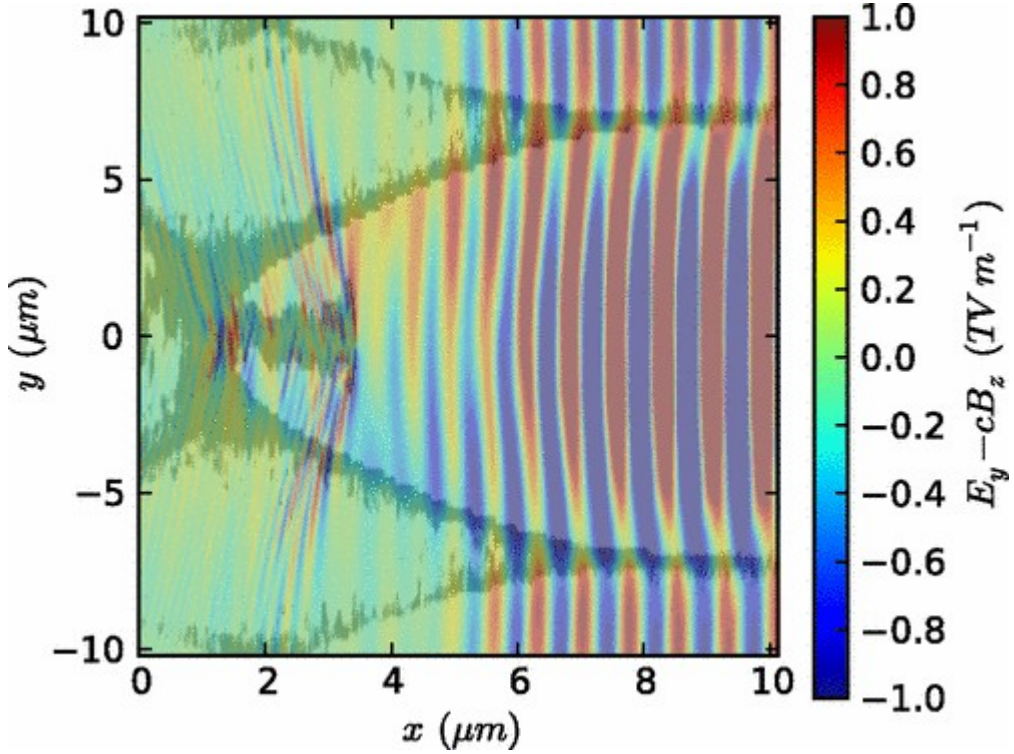
Rich and standardized description for physical quantities

Name	Value
axisLabels	[b'z' b'y' b'x']
dataOrder	b'C'
fieldSmoothing	b'none'
geometry	b'cartesian'
gridGlobalOffset	[0. 0. 0.]
gridSpacing	[4.252342 1.0630856 4.252342]
gridUnitSI	4.1671151662e-08
position	[0. 0. 0.]
timeOffset	0.0
unitDimension	[-3. 0. 1. 1. 0. 0. 0.]
unitSI	15399437.98944343

"The FAIR Guiding Principles for scientific data management and stewardship" (Mark D. Wilkinson et al.)

Extensions: e.g. ED-PIC

Field image → field solver, smoothing



similar:

Emittance → particle push, field solver, shape

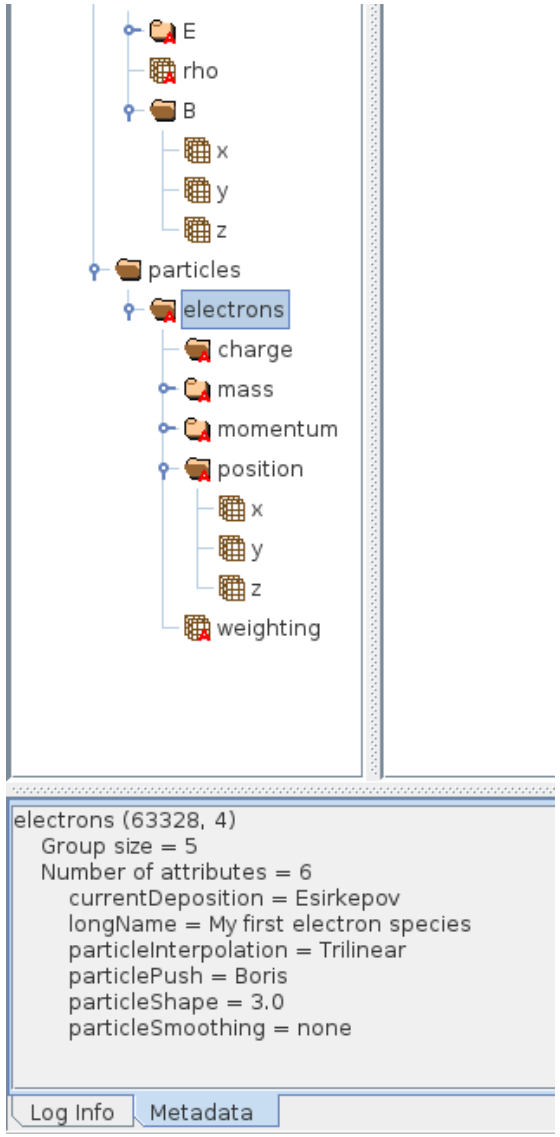


Image CC-BY 3.0: R. Lehe et al., RRSTAB 16, 021301 (2013), DOI:10.1103/PhysRevSTAB.16.021301

Modeling Mesh data

```
string    /data/1000/fields/E/axisLabels          attr   = {"z", "y", "x"}
string    /data/1000/fields/E/fieldSmoothing      attr   = "none"
string    /data/1000/fields/E/geometry            attr   = "cartesian"
double    /data/1000/fields/E/gridGlobalOffset    attr   = {0, 0, 0}
float     /data/1000/fields/E/gridSpacing         attr   = {4.25234, 1.06309, 4.25234}
double    /data/1000/fields/E/gridUnitSI          attr   = 4.16712e-08
float     /data/1000/fields/E/timeOffset          attr   = 0
double    /data/1000/fields/E/unitDimension       attr   = {1, 1, -3, -1, 0, 0, 0}
float     /data/1000/fields/E/x                   {192, 1536, 192} = 0 / 0
float     /data/1000/fields/E/x/position          attr   = {0.5, 0, 0}
double    /data/1000/fields/E/x/unitSI            attr   = 1.22627e+13
float     /data/1000/fields/E/y                   {192, 1536, 192} = 0 / 0
float     /data/1000/fields/E/y/position          attr   = {0, 0.5, 0}
double    /data/1000/fields/E/y/unitSI            attr   = 1.22627e+13
float     /data/1000/fields/E/z                   {192, 1536, 192} = 0 / 0
float     /data/1000/fields/E/z/position          attr   = {0, 0, 0.5}
double    /data/1000/fields/E/z/unitSI            attr   = 1.22627e+13
```

Mesh attributes, including fieldSmoothing defined by ED-PIC extension

x/y/z components for vector-type field (struct-of-array) including component-specific metadata

```
float     /data/1000/fields/e_all_energyDensity                    {192, 1536, 192} = 0 / 0
string    /data/1000/fields/e_all_energyDensity/axisLabels         attr   = {"z", "y", "x"}
string    /data/1000/fields/e_all_energyDensity/fieldSmoothing     attr   = "none"
string    /data/1000/fields/e_all_energyDensity/geometry           attr   = "cartesian"
double    /data/1000/fields/e_all_energyDensity/gridGlobalOffset   attr   = {0, 0, 0}
float     /data/1000/fields/e_all_energyDensity/gridSpacing        attr   = {4.25234, 1.06309, 4.25234}
double    /data/1000/fields/e_all_energyDensity/gridUnitSI         attr   = 4.16712e-08
float     /data/1000/fields/e_all_energyDensity/position           attr   = {0, 0, 0}
float     /data/1000/fields/e_all_energyDensity/timeOffset         attr   = 0
double    /data/1000/fields/e_all_energyDensity/unitDimension      attr   = {-1, 1, -2, 0, 0, 0, 0}
double    /data/1000/fields/e_all_energyDensity/unitSI             attr   = 7.8691e+12
```

Scalar-type field x/y/z layer is skipped

CASUS
CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

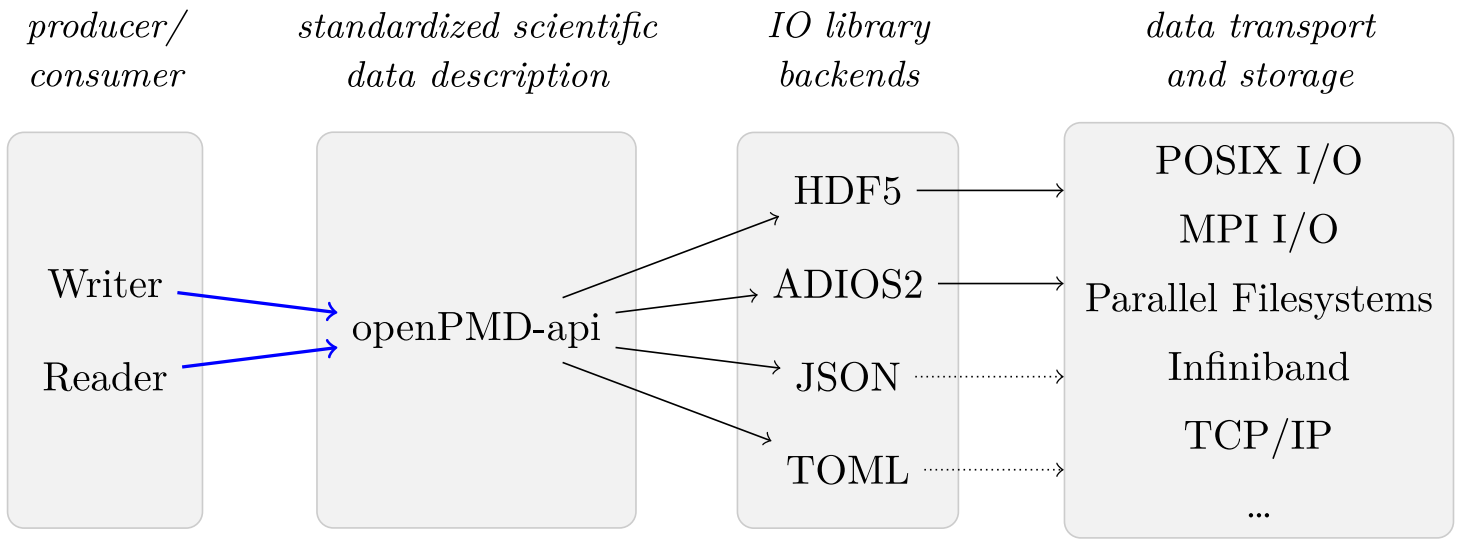
Hands-On:

openPMD-api: metadata

Module environment at `/project/project_465001310/workshop_software/env.sh`
Materials at `https://github.com/alpaka-group/alpaka-workshop-slides/tree/oct2024_workshop`

Read the `TODO` comments inside `src/openPMDOutput.hpp`:

openPMD-api – open stack for scientific I/O




```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, ...

CASUS
CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

Hands-On:

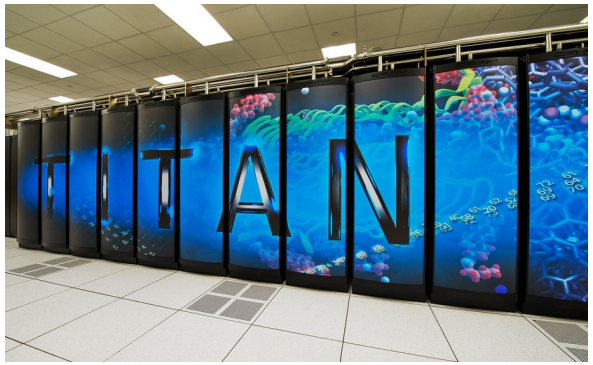
openPMD-api:

visualization, backend configuration

Module environment at `/project/project_465001310/workshop_software/env.sh`
Materials at `https://github.com/alpaka-group/alpaka-workshop-slides/tree/oct2024_workshop`
Launch Notebook at `https://www.lumi.csc.fi/`

Read the instructions inside `src/next_steps.md`:

Compute Performance Outpaces Storage Performance



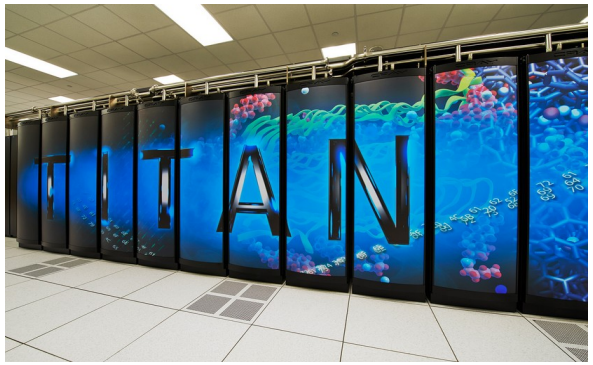
	Titan	Summit	Frontier	*Growth Factor*
Peak Performance:	27 Pflop/s	200 Pflop/s	1.6 Eflop/s	~60
FS Throughput:	1 TiByte/s	2.5 TiByte/s	5~10 TiByte/s	5~10
FS Capacity:	27 PiByte	250 PiByte	500~1000 PiByte	18~37

→ **parallel bandwidth** insufficient for HPC at full scale
→ **filesystem capacity** insufficient for HPC at full scale

Same trend in **experiments**?
→ Increasing **camera resolutions and data rates**

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.

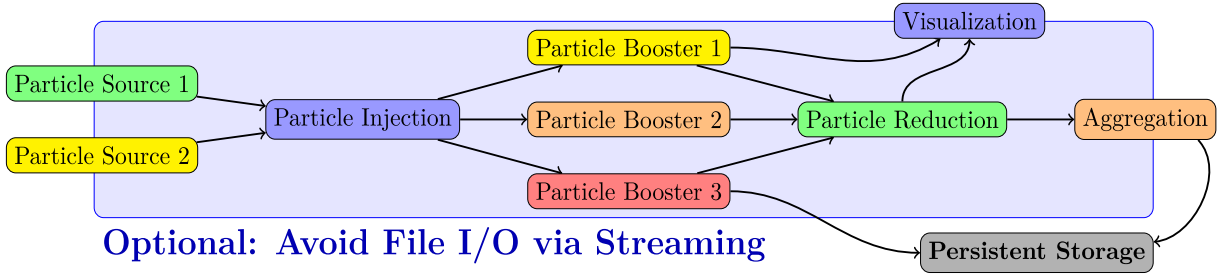
Compute Performance Outpaces Storage Performance



	Titan	Summit	Frontier	Growth Factor
Peak Performance:	27 Pflop/s	200 Pflop/s	1.6 Eflop/s	~60
FS Throughput:	1 TiByte/s	2.5 TiByte/s	5~10 TiByte/s	5~10
FS Capacity:	27 PiByte	250 PiByte	500~1000 PiByte	18~37

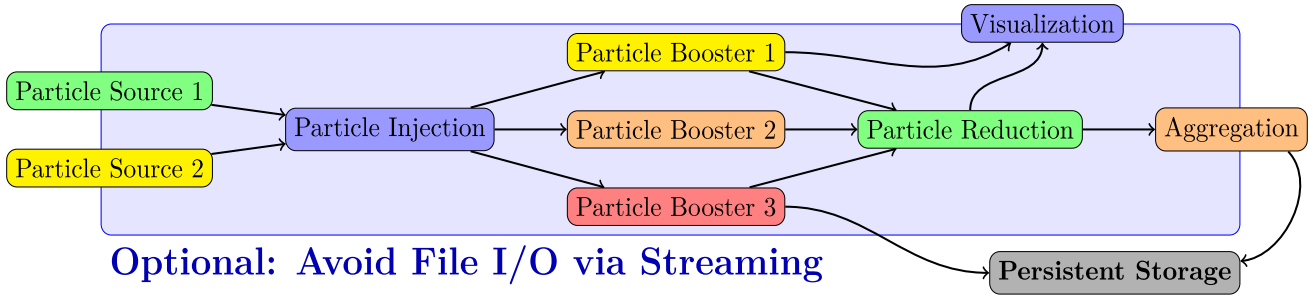
Why does this concern us?

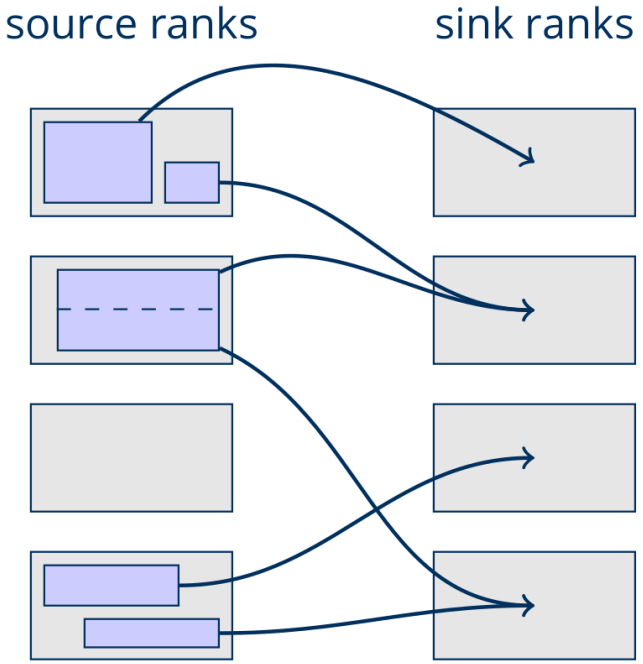
- Heterogeneous data processing pipelines traditionally have large I/O usage
- Scalable alternative: Streaming



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.

Streaming: Don’t touch the Filesystem at all



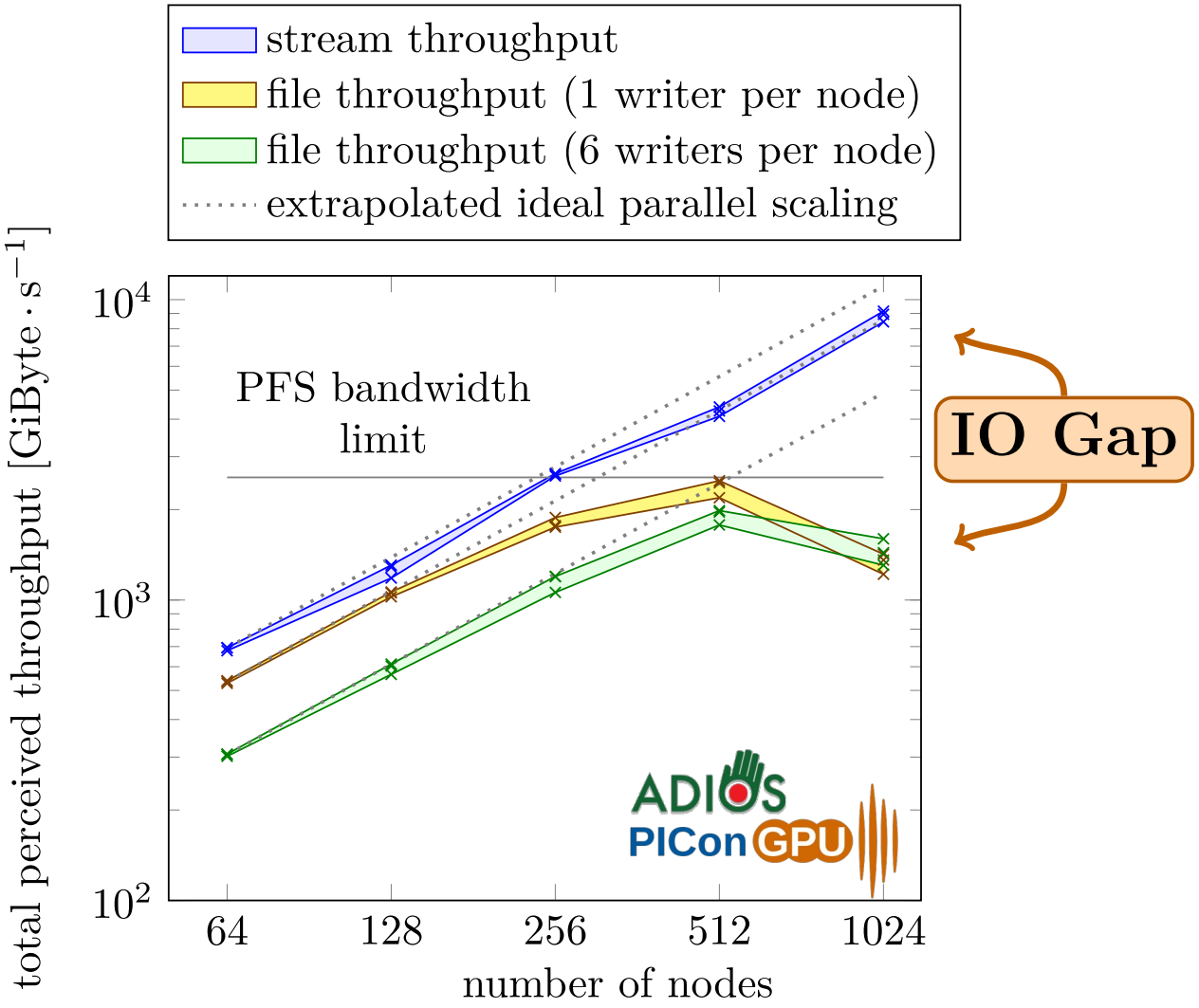


- Data processing pipelines and increasingly experiments setups have large I/O usage
- Scalable alternative: Streaming
  e.g. via Infiniband (on HPC systems)
  or wide area networks (in lab settings)

Challenge:
Compute a balanced, aligned, local mapping between two applications that remains useful in the problem domain

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

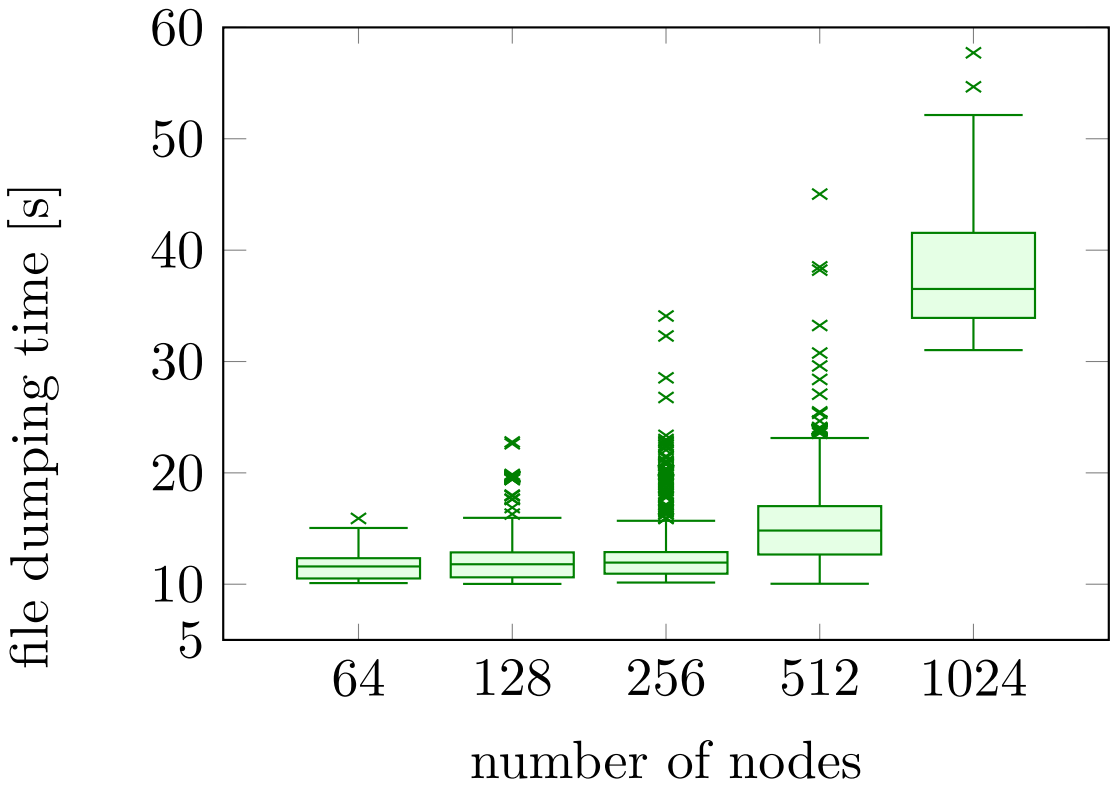


Memory-bound simulations reach the I/O system limits at a fraction of full scale

- Summit FS bandwidth (2.5TiByte/s) reached at 512 nodes (~11% of system size)
- Streaming workflows unaffected by filesystem bandwidth, use Infiniband hardware to scale beyond it

(benchmarks at 1024 nodes done after Summit system upgrade)

Summit: Performance fluctuations on single ranks



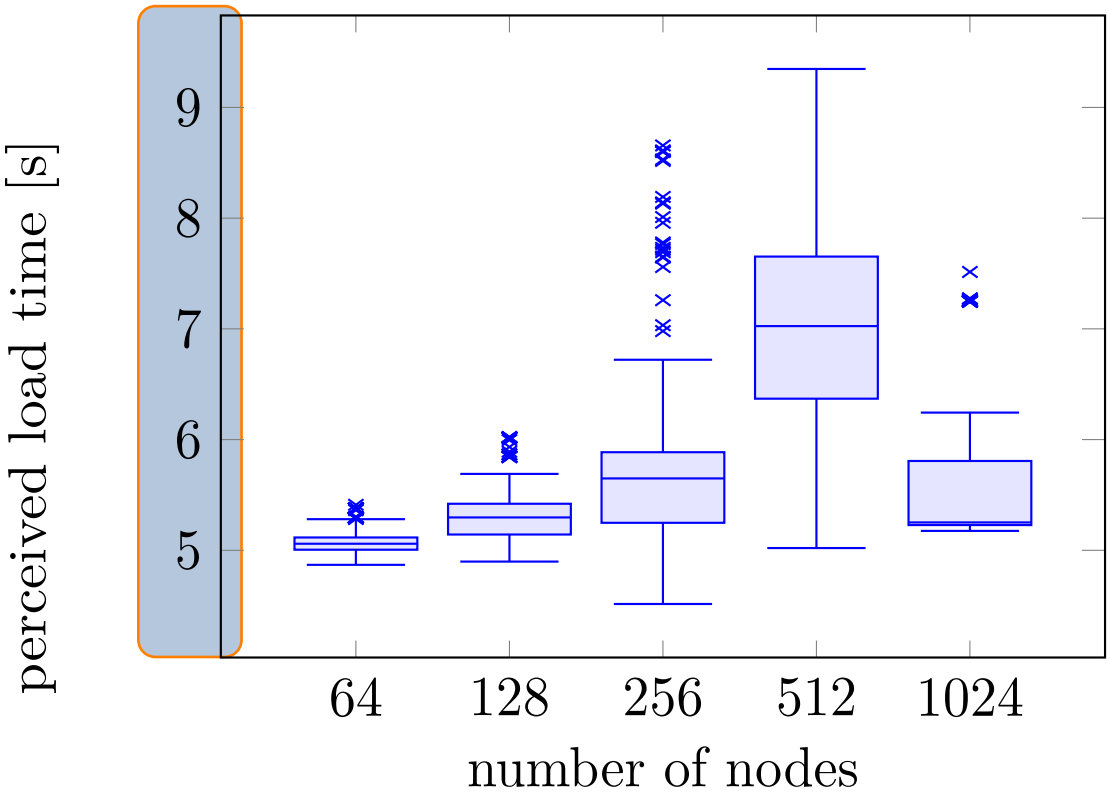
Same results, different display:

- Plot every single measurement
- Visualize reproducibility
- Box: 50% of measurement points
- Whiskers: “normal” measurements
- Others: outliers

Evaluation for file-only setup:

- Median time slightly raised at 512 nodes
  Scaling stops due to PFS limit after that
- Outliers increasing with scale
- Outliers fatal in parallel contexts

Summit: Well-reproducible performance of Infiniband Streaming



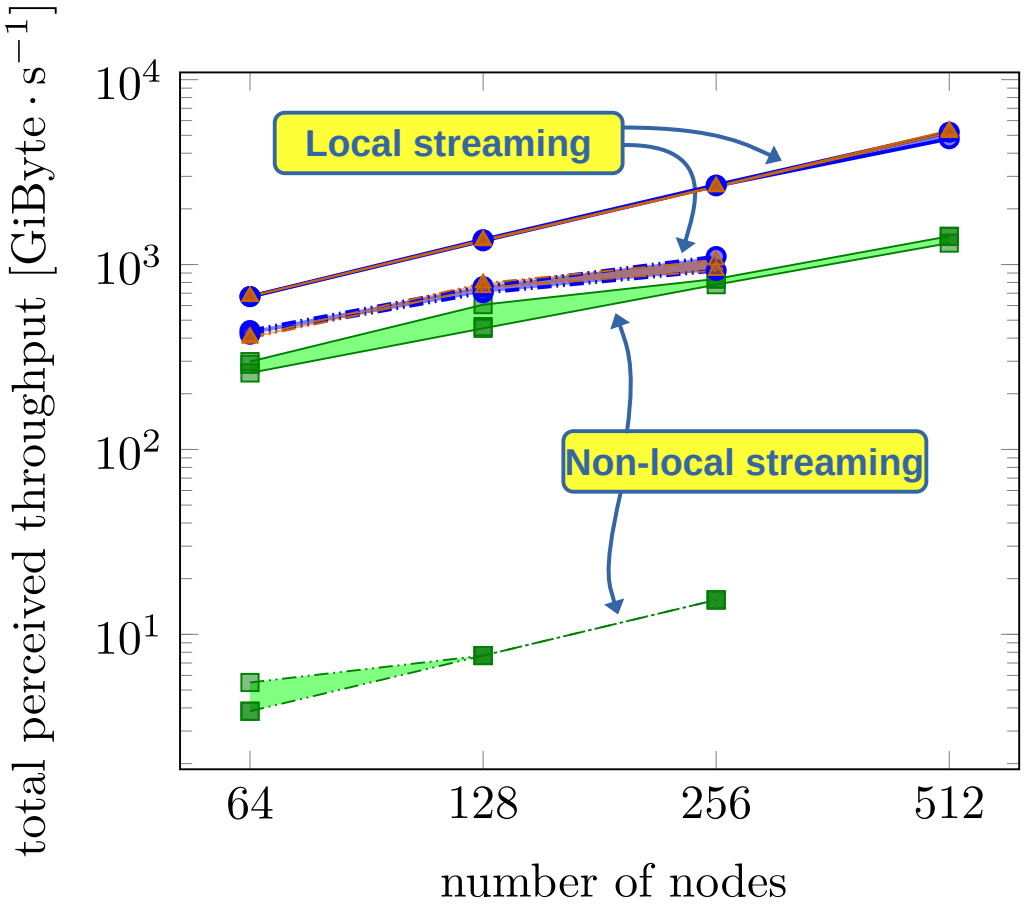
Same results, different display:

- Plot every single measurement
- Visualize reproducibility
- Box: 50% of measurement points
- Whiskers: “normal” measurements
- Others: outliers

stream+file setup (stream part):

- Overall times are lower
- Median between 5 and 7 seconds
- Outliers less dominating by far

For good throughput:
Local streaming patterns, Infiniband/RDMA



Local streaming:

Distribute data chunks only within a node

Non-local streaming:

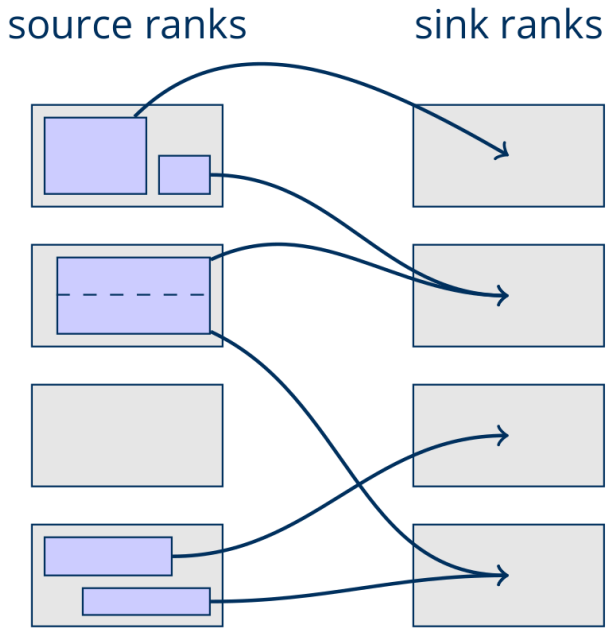
Distribute data chunks globally, optimize for balance and alignment

Straight lines:

Infiniband/RDMA

Dashed lines:

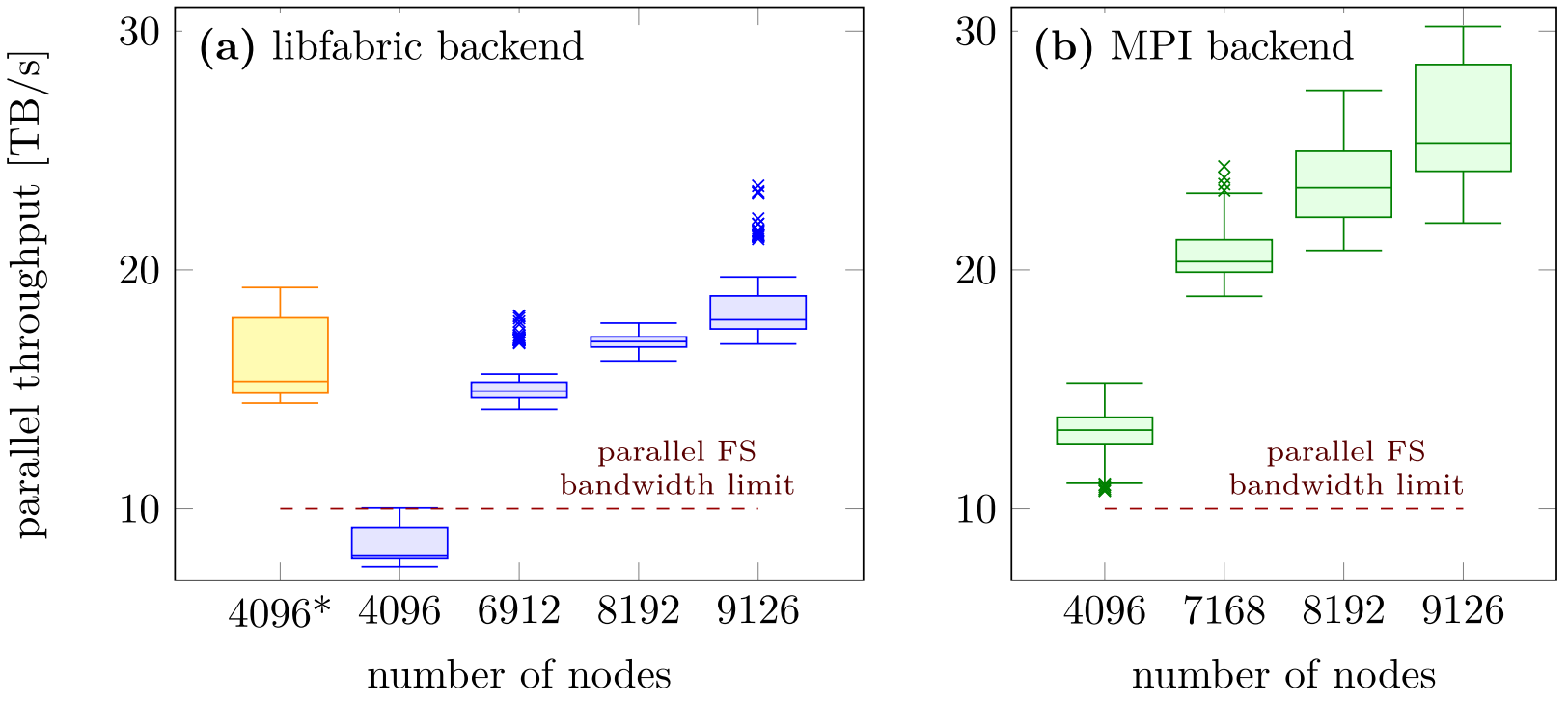
TCP/sockets



Setup: Couple PIConGPU with a scattering code (GAPD) exchange particle data only

J. C. E, L. Wang, S. Chen, Y. Y. Zhang and S. N. Luo. “GAPD: a GPU- accelerated atom-based polychromatic diffraction simulation code”. In: Journal of Synchrotron Radiation 25.2 (Mar. 2018), pp. 604–611.

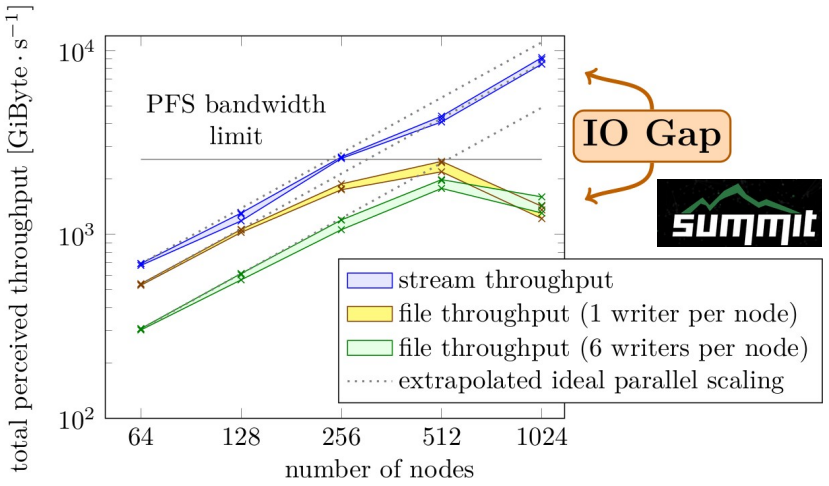
Break through Filesystem Bandwidth with Streaming



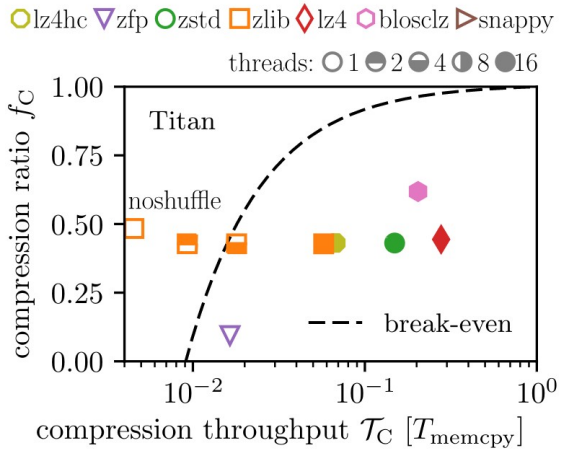
Full scale of Frontier:

Leaving behind us
the theoretical bandwidth
of the parallel filesystem

Performance: Data Layouts and no-file I/O

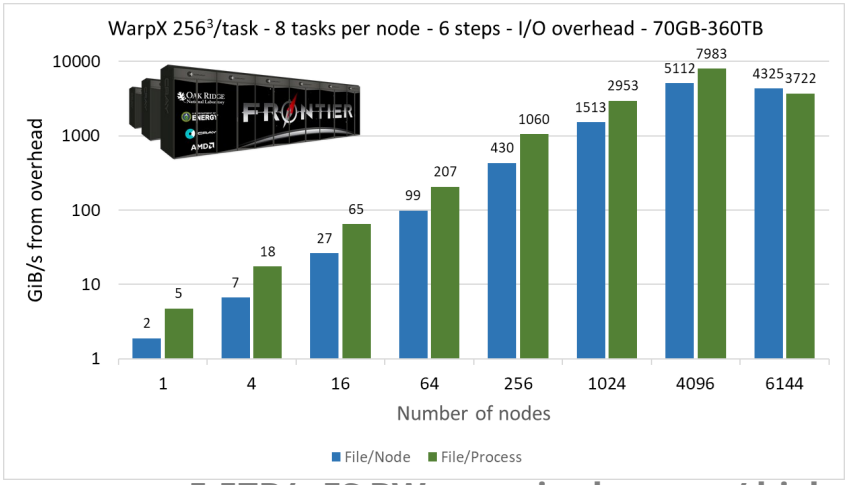


Streaming Data Pipelines:
DOI:10.1007/978-3-030-96498-6_6
by F Poeschel, A Huebl et al., SMC21 (2022)



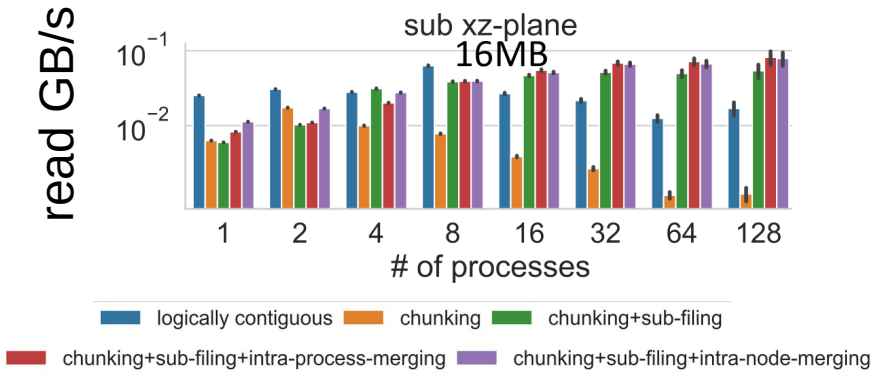
Fast Compressors Needed:
DOI:10.1007/978-3-319-67630-2_2
by A Huebl et al., ISC DRBSD-1 (2017)

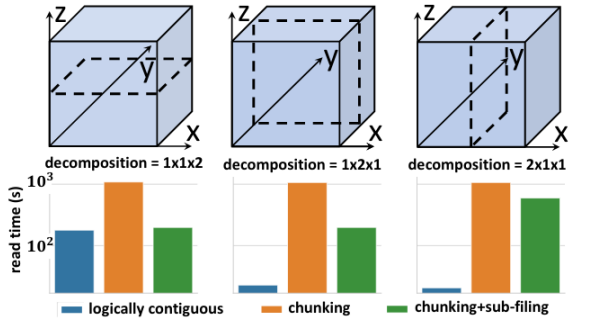
openPMD-api w/ WarpX



>5.5TB/s FS BW: two-tier lustre w/ high-performance storage & progressive files

Online Data Layout Reorganization:
DOI:10.1109/TPDS.2021.3100784
by L Wan, A Huebl et al., TPDS (2021)





Impact of decomposition schemes when reading

CASUS
CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

Hands-On:

openPMD-api:

streaming I/O

Module environment at `/project/project_465001310/workshop_software/env.sh`
Materials at `https://github.com/alpaka-group/alpaka-workshop-slides/tree/oct2024_workshop`
Launch Notebook at `https://www.lumi.csc.fi/`

Read the instructions inside `src/visualize.py` (open as a Jupyter Notebook):

openPMD powered Projects and Users

Documents:

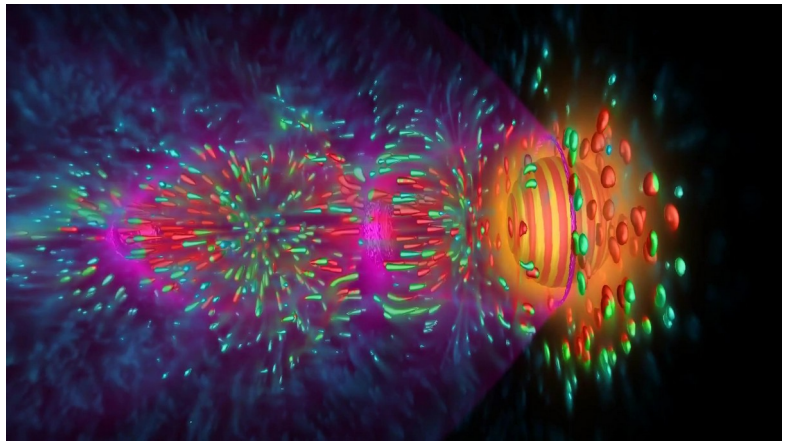
- **openPMD standard** (1.0.0, 1.0.1, 1.1.0)
  the underlying file markup and definition
  A Huebl et al., doi: 10.5281/zenodo.33624

Language Binding:

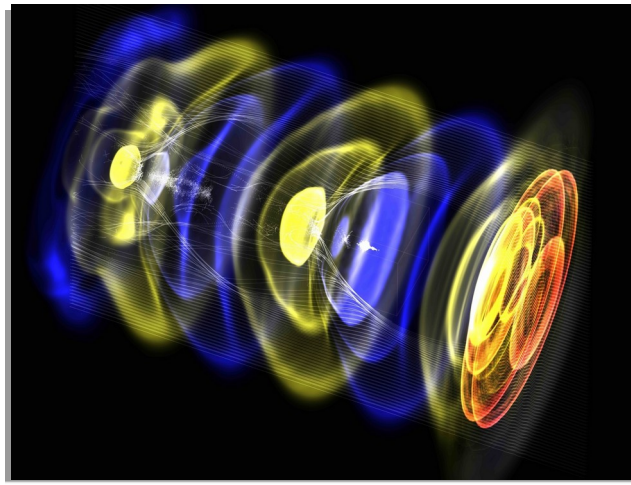
- **openPMD-api** (HZDR, CASUS, LBNL)
  reference API for openPMD data handling
  maintainers: A Huebl, J Gu, F Poeschel et al.

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

openPMD powered Projects and Users

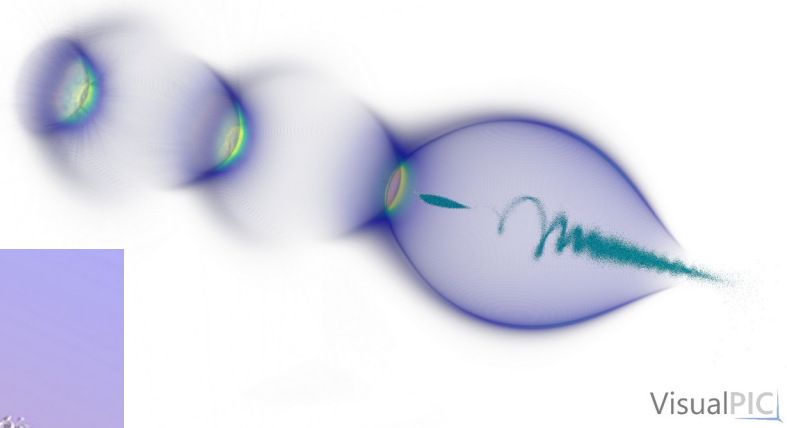
Documents:

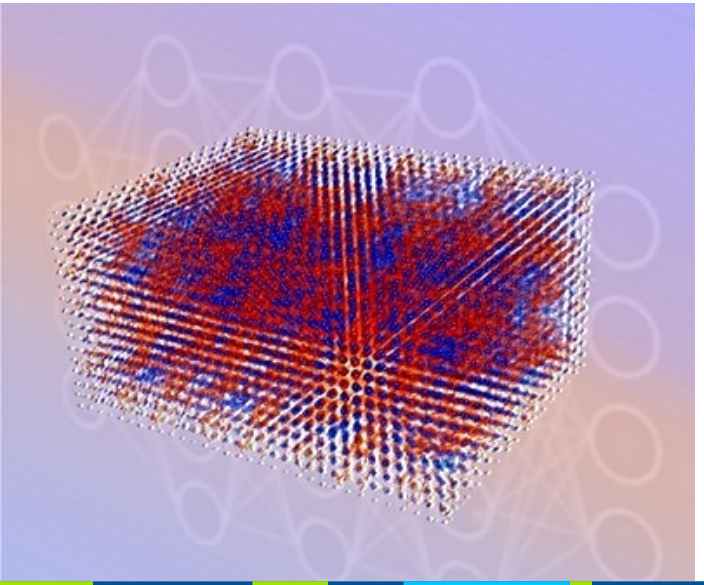
- **openPMD standard** (1.0.0, 1.0.1, 1.1.0)
  the underlying file markup and definition
  A Huebl et al., doi: 10.5281/zenodo.33624

Language Binding:

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

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...

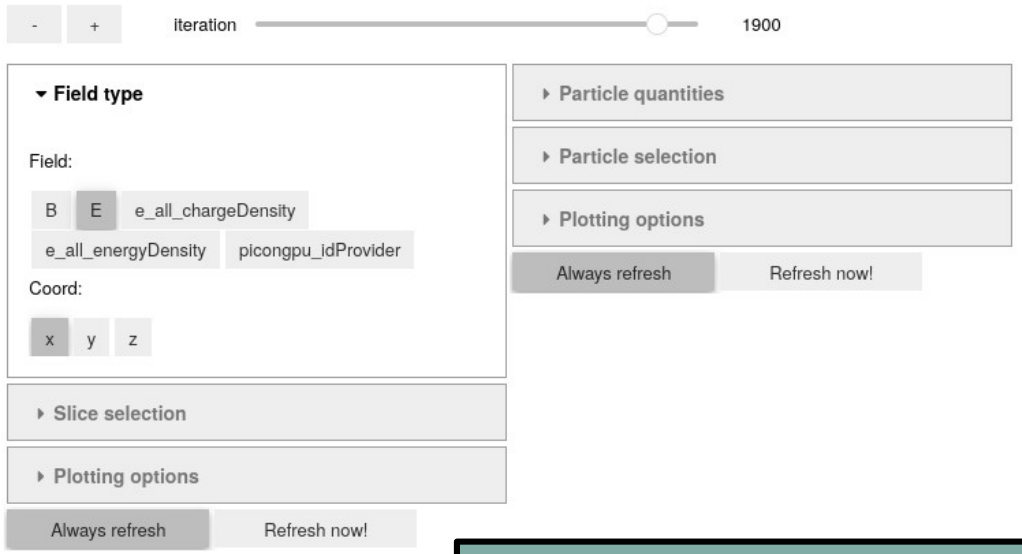
see also: https://github.com/openPMD/openPMD-projects

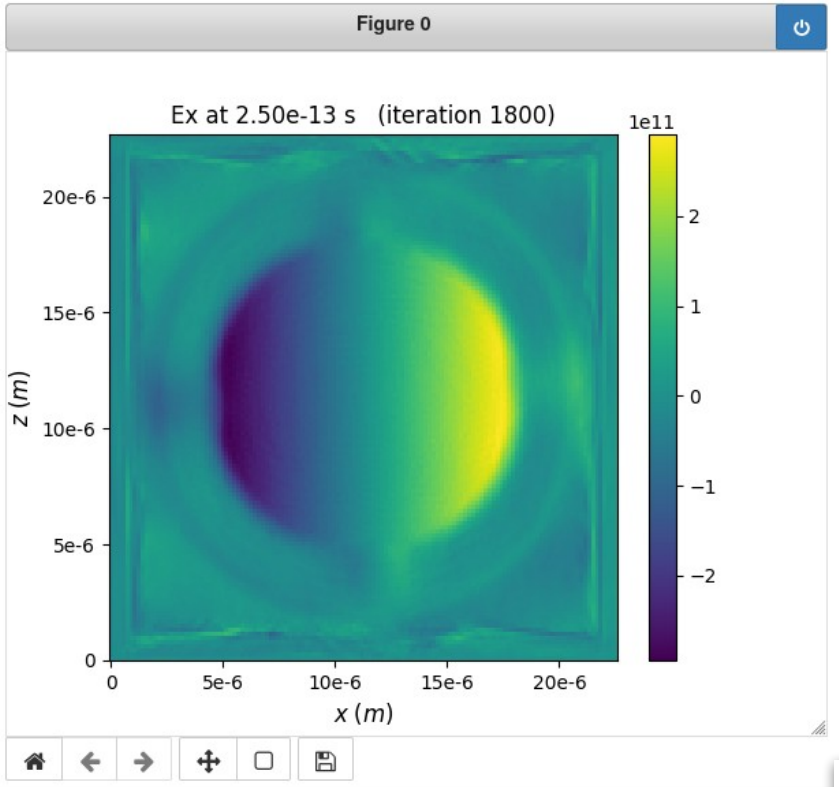
Analysis and Visualization

```
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()
```

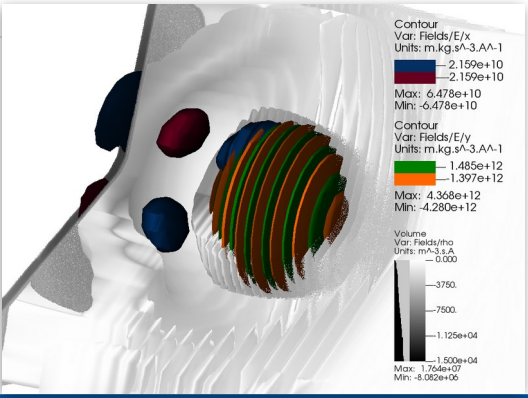




openPMD/openPMD-viewer

Standardization of data

→ integration into modern scientific compute workflows



Hands-On:

openPMD-viewer:

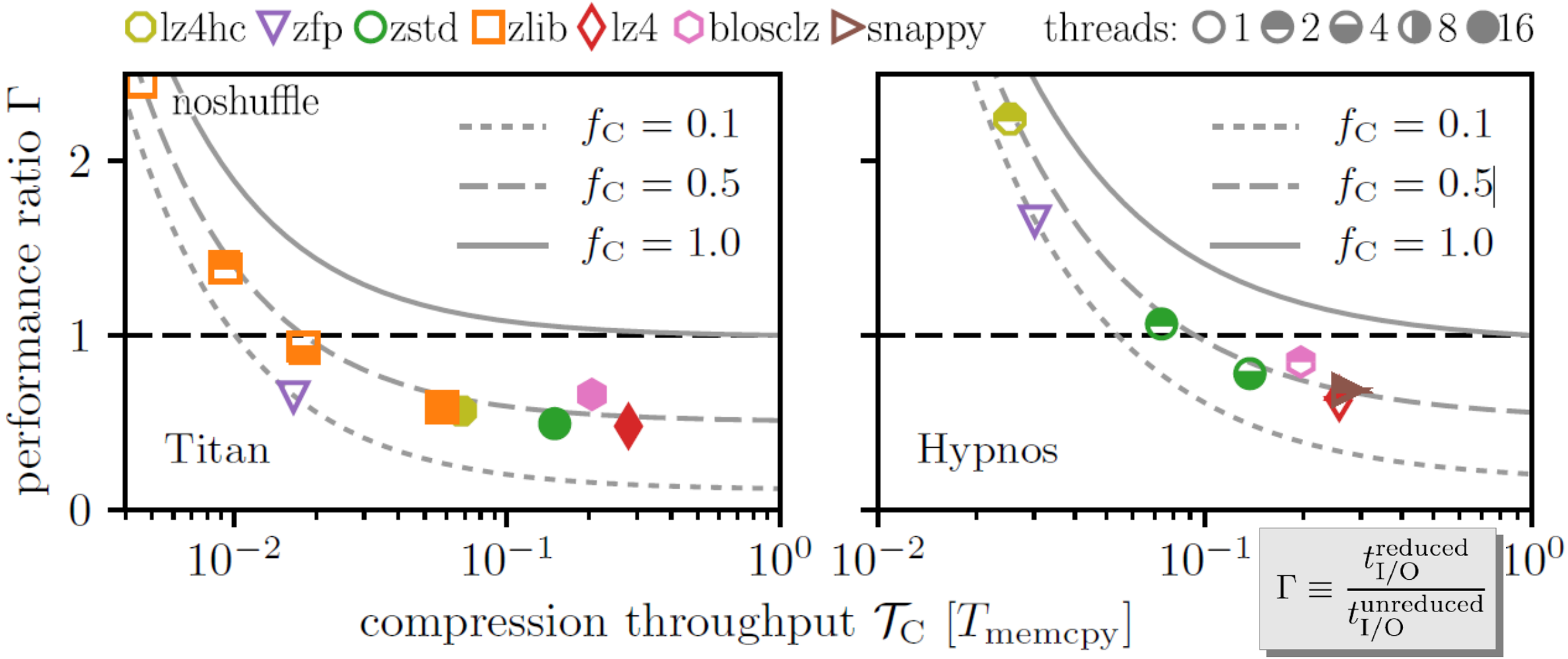
visualizing data written by
a PIConGPU LaserWakefield simulation

Module environment at `/project/project_465001310/workshop_software/env.sh`
Materials at `https://github.com/alpaka-group/alpaka-workshop-slides/tree/oct2024_workshop`
Launch Notebook at `https://www.lumi.csc.fi/`

Read the instructions inside `next_steps.md`:

Data-driven Science

Just compress the data and everything will be fine …?



A. Huebl et al., "On the Scalability of Data Reduction Techniques in Current and Upcoming HPC Systems from an Application Perspective", In: Lect. Notes Comput. Sci. 10524.4, pp.15-20 (2017)

Hands-On:

compression

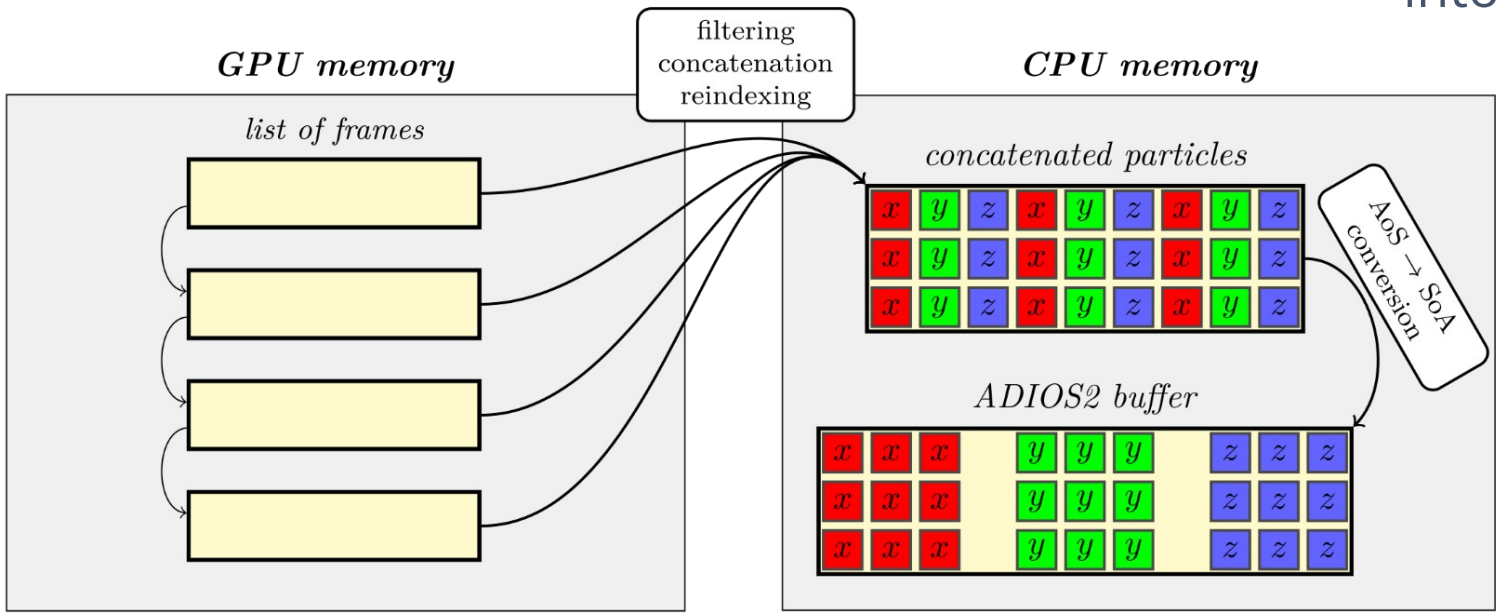
Module environment at `/project/project_465001310/workshop_software/env.sh`
Materials at `https://github.com/alpaka-group/alpaka-workshop-slides/tree/oct2024_workshop`
Launch Notebook at `https://www.lumi.csc.fi/`

Continue with the instructions in the openPMD-viewer Notebook

Data path in a realistic application

- In real-world applications, data is often kept in a custom, algorithm-driven format
- Reorganization needed before output

- However: ADIOS2 (optionally) buffers data before output for I/O performance
- Few big operations better than many small operations
- Elide one data copy by writing directly into those internal buffers



Example:

Transforming PIConGPU particle data for output

CASUS
CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

Advanced Hands-On:

openPMD-api:

Span API

Module environment at `/project/project_465001310/workshop_software/env.sh`
Materials at `https://github.com/alpaka-group/alpaka-workshop-slides/tree/oct2024_workshop`
Launch Notebook at `https://www.lumi.csc.fi/`

Read the instructions inside `src/openPMDOutput.hpp`

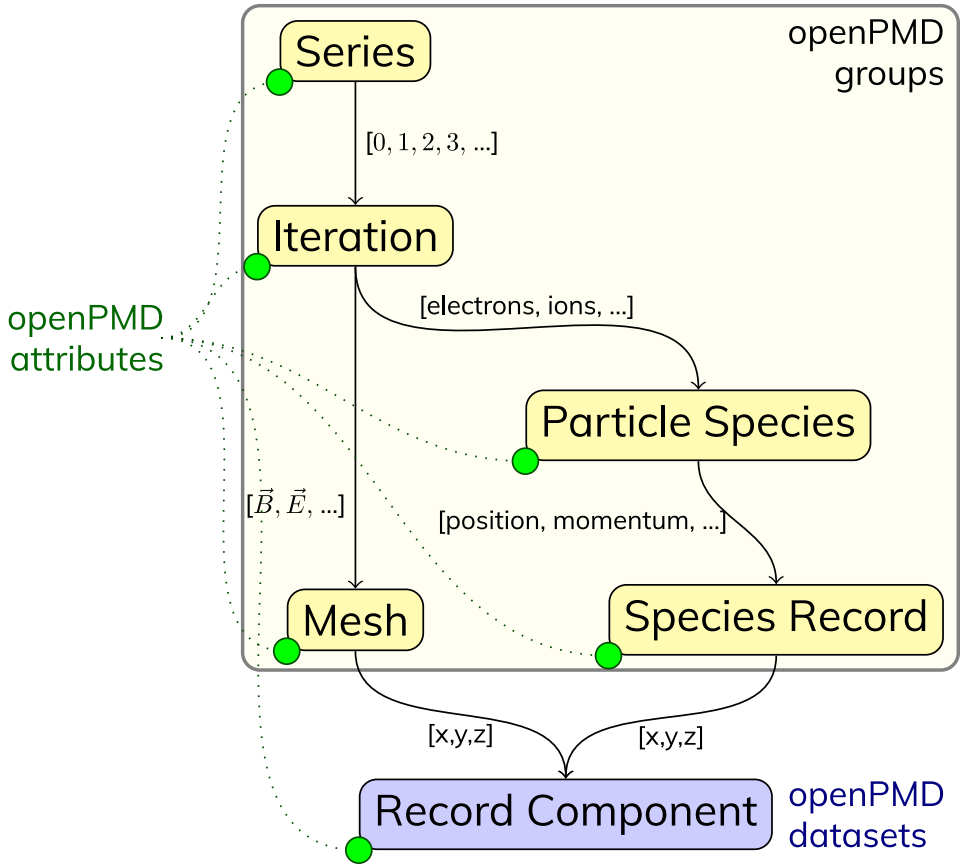
Modeling particle data

```
uint32_t  /data/particles/e/position/macroWeighted          attr   = 0
float     /data/particles/e/position/timeOffset             attr   = 0
double    /data/particles/e/position/unitDimension          attr   = {1, 0, 0, 0, 0, 0, 0}
double    /data/particles/e/position/weightingPower         attr   = 0
float     /data/particles/e/position/x                      {109134176} = 0 / 0
double    /data/particles/e/position/x/unitSI               attr   = 1.772e-07
float     /data/particles/e/position/y                      {109134176} = 0 / 0
double    /data/particles/e/position/y/unitSI               attr   = 4.43e-08
float     /data/particles/e/position/z                      {109134176} = 0 / 0
double    /data/particles/e/position/z/unitSI               attr   = 1.772e-07

uint32_t  /data/particles/e/positionOffset/macroWeighted    attr   = 0
float     /data/particles/e/positionOffset/timeOffset       attr   = 0
double    /data/particles/e/positionOffset/unitDimension    attr   = {1, 0, 0, 0, 0, 0, 0}
double    /data/particles/e/positionOffset/weightingPower   attr   = 0
int32_t   /data/particles/e/positionOffset/x                {109134176} = 0 / 0
double    /data/particles/e/positionOffset/x/unitSI         attr   = 1.772e-07
int32_t   /data/particles/e/positionOffset/y                {109134176} = 0 / 0
double    /data/particles/e/positionOffset/y/unitSI         attr   = 4.43e-08
int32_t   /data/particles/e/positionOffset/z                {109134176} = 0 / 0
double    /data/particles/e/positionOffset/z/unitSI         attr   = 1.772e-07

float     /data/particles/e/weighting                       {109134176} = 0 / 0
uint32_t  /data/particles/e/weighting/macroWeighted         attr   = 1
float     /data/particles/e/weighting/timeOffset            attr   = 0
double    /data/particles/e/weighting/unitDimension         attr   = {0, 0, 0, 0, 0, 0, 0}
double    /data/particles/e/weighting/unitSI                attr   = 1
double    /data/particles/e/weighting/weightingPower        attr   = 1
```

Let's have a detailed look at the electron species written by PIConGPU…



Modeling particle data: mandatory records, vector vs. scalar

```
uint32_t  /data/particles/e/position/macroWeighted          attr   = 0
float     /data/particles/e/position/timeOffset             attr   = 0
double    /data/particles/e/position/unitDimension          attr   = {1, 0, 0, 0, 0, 0, 0}
double    /data/particles/e/position/weightingPower         attr   = 0
float     /data/particles/e/position/x                      {109134176} = 0 / 0
double    /data/particles/e/position/x/unitSI               attr   = 1.772e-07
float     /data/particles/e/position/y                      {109134176} = 0 / 0
double    /data/particles/e/position/y/unitSI               attr   = 4.43e-08
float     /data/particles/e/position/z                      {109134176} = 0 / 0
double    /data/particles/e/position/z/unitSI               attr   = 1.772e-07

uint32_t  /data/particles/e/positionOffset/macroWeighted    attr   = 0
float     /data/particles/e/positionOffset/timeOffset       attr   = 0
double    /data/particles/e/positionOffset/unitDimension    attr   = {1, 0, 0, 0, 0, 0, 0}
double    /data/particles/e/positionOffset/weightingPower   attr   = 0
int32_t   /data/particles/e/positionOffset/x                {109134176} = 0 / 0
double    /data/particles/e/positionOffset/x/unitSI         attr   = 1.772e-07
int32_t   /data/particles/e/positionOffset/y                {109134176} = 0 / 0
double    /data/particles/e/positionOffset/y/unitSI         attr   = 4.43e-08
int32_t   /data/particles/e/positionOffset/z                {109134176} = 0 / 0
double    /data/particles/e/positionOffset/z/unitSI         attr   = 1.772e-07

float     /data/particles/e/weighting                       {109134176} = 0 / 0
uint32_t  /data/particles/e/weighting/macroWeighted         attr   = 1
float     /data/particles/e/weighting/timeOffset            attr   = 0
double    /data/particles/e/weighting/unitDimension         attr   = {0, 0, 0, 0, 0, 0, 0}
double    /data/particles/e/weighting/unitSI                attr   = 1
double    /data/particles/e/weighting/weightingPower        attr   = 1
```

position: mandatory record for particles

position is a vector quantity, i.e. has x/y/z
struct-of-array-like layout:
3 vectors of same length

positionOffset: also mandatory
specifies the base for the position
used for numerical reasons

weighting: custom record in PIConGPU
to model macro particles
scalar quantity, x/y/z is skipped

Modeling particle data: constant components

```
string    /data/particles/e/currentDeposition          attr   = "Esirkepov"
string    /data/particles/e/particleInterpolation      attr   = "uniform"
string    /data/particles/e/particlePush               attr   = "Boris"
double    /data/particles/e/particleShape              attr   = 2
string    /data/particles/e/particleSmoothing          attr   = "none"

int32_t   /data/particles/e/charge/macroWeighted       attr   = 0
uint64_t  /data/particles/e/charge/shape               attr   = {109134176}
double    /data/particles/e/charge/timeOffset          attr   = 0
double    /data/particles/e/charge/unitDimension       attr   = {0, 0, 1, 1, 0, 0, 0}
double    /data/particles/e/charge/unitSI              attr   = 1.11432e-15
double    /data/particles/e/charge/value               attr   = -0.00014378
double    /data/particles/e/charge/weightingPower      attr   = 1

int32_t   /data/particles/e/mass/macroWeighted         attr   = 0
uint64_t  /data/particles/e/mass/shape                 attr   = {109134176}
double    /data/particles/e/mass/timeOffset            attr   = 0
double    /data/particles/e/mass/unitDimension         attr   = {0, 1, 0, 0, 0, 0, 0}
double    /data/particles/e/mass/unitSI                attr   = 6.33564e-27
double    /data/particles/e/mass/value                 attr   = 0.00014378
double    /data/particles/e/mass/weightingPower        attr   = 1

uint32_t  /data/particles/e/momentum/macroWeighted     attr   = 1
float     /data/particles/e/momentum/timeOffset        attr   = 0
double    /data/particles/e/momentum/unitDimension     attr   = {1, 1, -1, 0, 0, 0, 0}
double    /data/particles/e/momentum/weightingPower    attr   = 1
float     /data/particles/e/momentum/x                 {109134176} = 0 / 0
double    /data/particles/e/momentum/x/unitSI          attr   = 1.89938e-18
float     /data/particles/e/momentum/y                 {109134176} = 0 / 0
double    /data/particles/e/momentum/y/unitSI          attr   = 1.89938e-18
float     /data/particles/e/momentum/z                 {109134176} = 0 / 0
double    /data/particles/e/momentum/z/unitSI          attr   = 1.89938e-18
```

particle attributes defined
by the ED-PIC extension

charge and mass:
are fixed for one particle species,
i.e. record has one constant value
→ define via attributes `shape` and `value`
instead of writing the whole array
scalar quantities as well

momentum:
again a non-constant
vector quantity

Modeling particle data: particle patches

```
uint64_t  /data/1000/particles/e/particlePatches/offset/x                {8}
  (0)    0 0 0 0 96 96 96 96

uint64_t  /data/1000/particles/e/particlePatches/offset/y                {8}
  (0)    0 512 1024 1536 0 512 1024 1536

uint64_t  /data/1000/particles/e/particlePatches/offset/z                {8}
  (0)    0 0 0 0 0 0 0 0

uint64_t  /data/1000/particles/e/particlePatches/extent/x                {8}
  (0)    96 96 96 96 96 96 96 96

uint64_t  /data/1000/particles/e/particlePatches/extent/y                {8}
  (0)    512 512 512 0 512 512 512 0

uint64_t  /data/1000/particles/e/particlePatches/extent/z                {8}
  (0)    192 192 192 192 192 192 192 192


uint64_t  /data/1000/particles/e/particlePatches/numParticlesOffset      {8}
  (0)    0 16916087 35692896 54567264 54567264 71482787 90259808 109134176

uint64_t  /data/1000/particles/e/particlePatches/numParticles            {8}
  (0)    16916087 18776809 18874368 0 16915523 18777021 18874368 0
```

green: GPU 0

Common case: Each GPU computes one sub-areal of the global simulation space

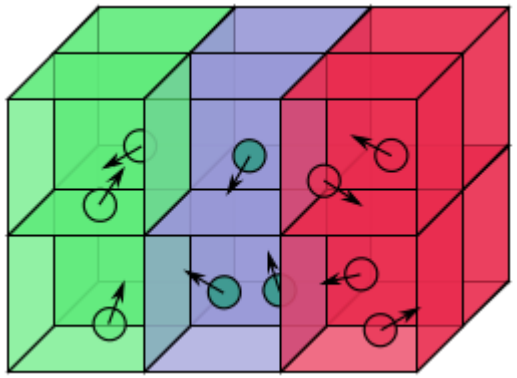
→ Particles are written in patches, each GPU's patch is spatially bounded

- offset/extent define the box wherein the particles are located
- numParticlesOffset/numParticles define the patch's position in the list

e.g.: GPU 0 computes the box (0, 0, 0)–(96, 512, 192) (in simulation units),

its electron data is found from index 0 to 16916087

Note: extent is always relative to the offset



CASUS
CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

Advanced Hands-On:

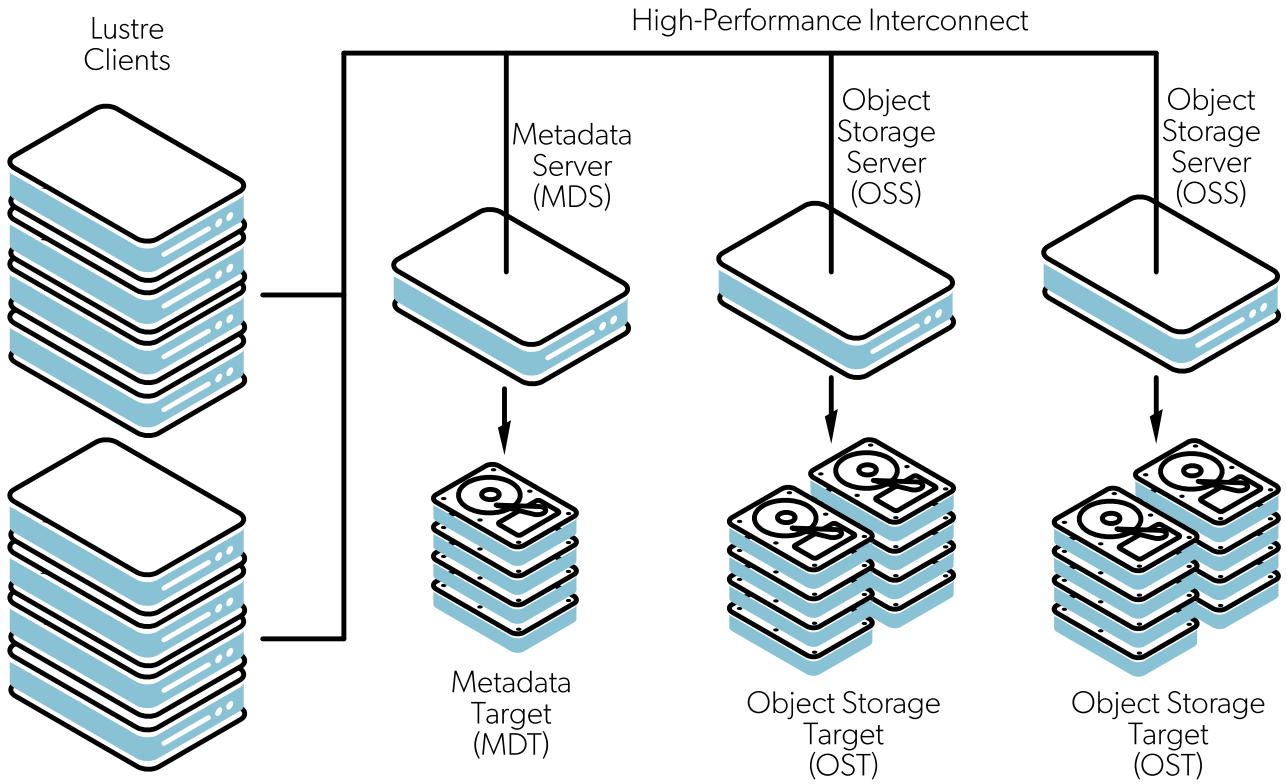
openPMD-api:

Python API: constant components

Module environment at `/project/project_465001310/workshop_software/env.sh`
Materials at `https://github.com/alpaka-group/alpaka-workshop-slides/tree/oct2024_workshop`
Launch Notebook at `https://www.lumi.csc.fi/`

Read the TODO comments inside `write_parallel.py`

Using parallel filesystems

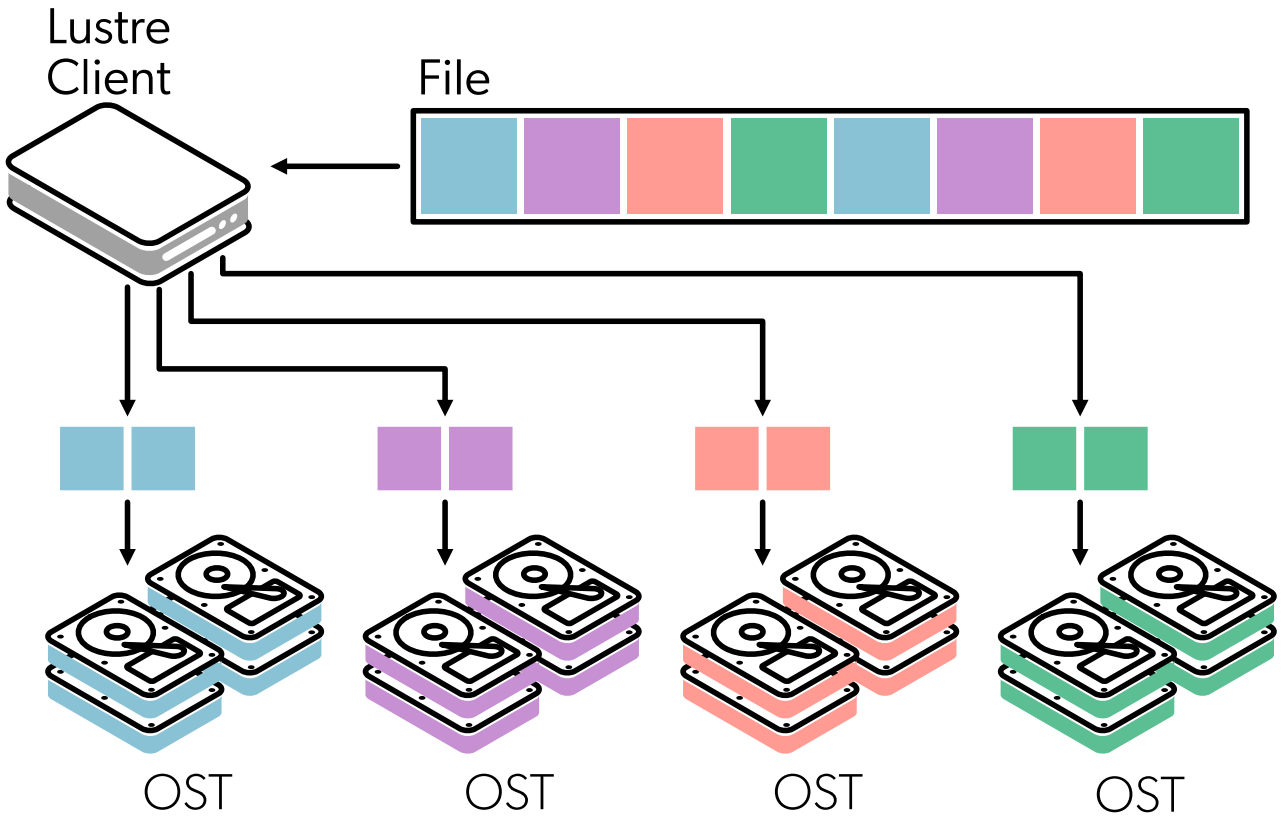


Lumi uses Lustre,
a popular parallel filesystem

- Parallel filesystems are built from distributed hardware
- One ore more metadata servers manage one or more metadata targets
- Many object storage servers manage each one or more object storage targets
- Key to I/O performance:
  Use the parallel resources
  (but mind that they are shared with other users)

Image from
https://docs.lumi-supercomputer.eu/storage/parallel-filesystems/lustre/

File striping – an approach at parallel I/O performance



Write file in parallel by striping it across multiple OSTs

- `stripe_size` sets the homogeneous length of each stripe
- `stripe_count` sets the number of used OSTs

Main use:

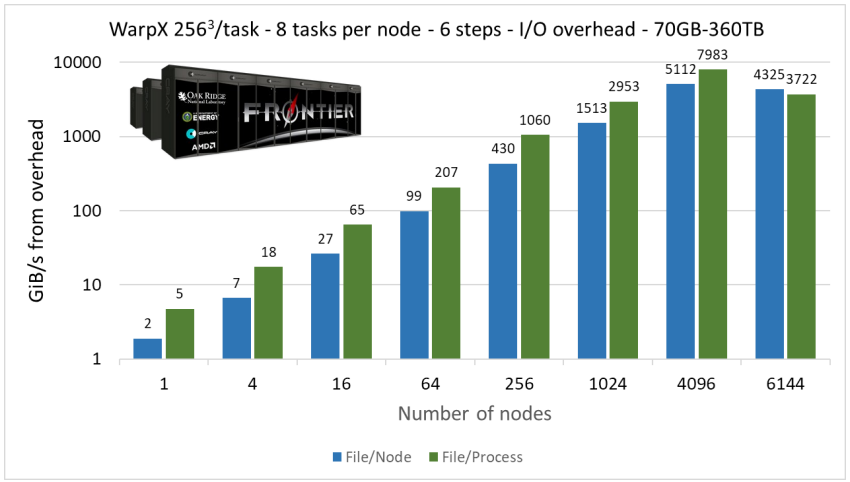
- Improving speed of serial I/O
- Improving speed of parallel I/O to a single file
- At low scale: Improving speed of parallel I/O to multiple files

Better: Write multiple files from the start already → Subfiling

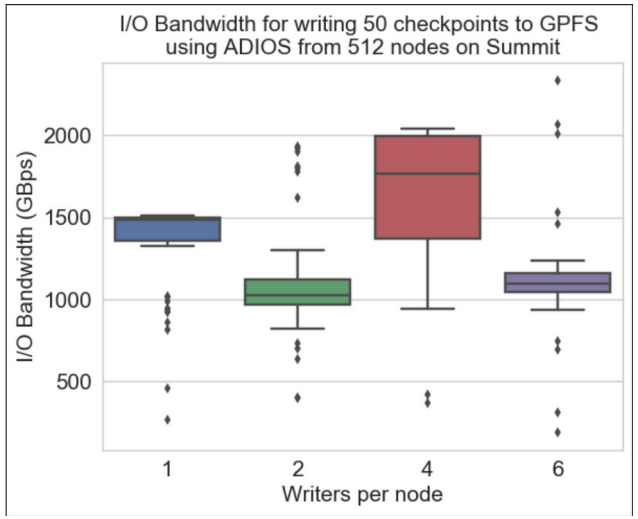
Image from
https://docs.lumi-supercomputer.eu/storage/parallel-filesystems/lustre/

Subfiling – key for performance at full scale

openPMD-api w/ WarpX



>5.5TB/s FS BW: two-tier lustre w/ high-performance storage & progressive files



Subfiling is NOT independent I/O

- Mapping processes to files N:1 scales badly
- Mapping processes to files N:N scales up to a mediocre size, then overloads the filesystem
- Subfiling: N:M mapping where M≤N
- Many different aggregation schemes in ADIOS2 and HDF5, one size does not fit all

ADIOS2: Aggregate to one writer per node by default

HDF5: Complex N→N aggregation scheme due to structured output to disk

L. Wan et al.: Data Management Challenges of Exascale Scientific Simulations: A Case Study with the Gyrokinetic Toroidal Code and ADIOS

CASUS
CENTER FOR ADVANCED SYSTEMS UNDERSTANDING

Advanced Hands-On:

openPMD-api:

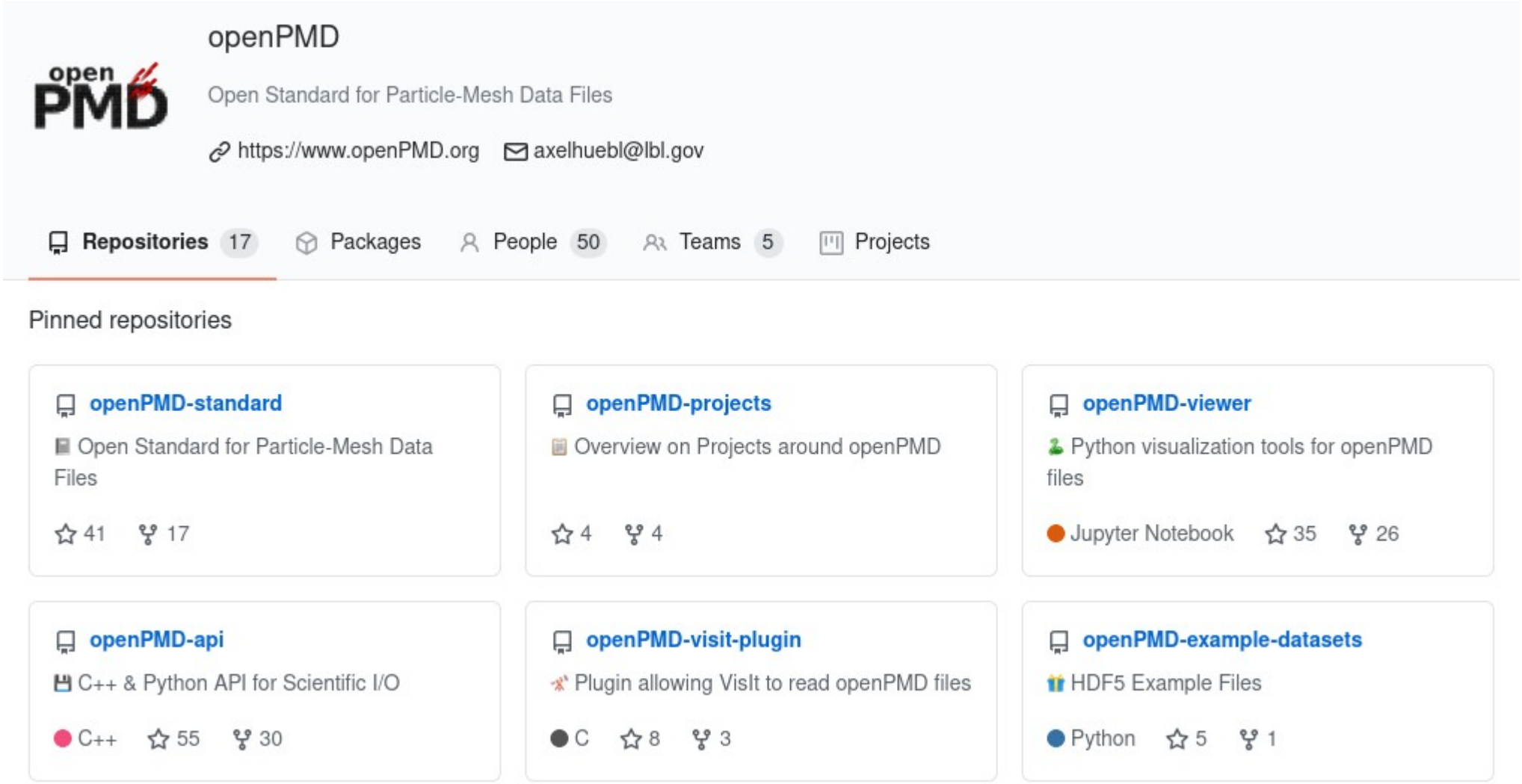
Python API: Parallel Writing

Module environment at `/project/project_465001310/workshop_software/env.sh`
Materials at `https://github.com/alpaka-group/alpaka-workshop-slides/tree/oct2024_workshop`
Launch Notebook at `https://www.lumi.csc.fi/`

Read the TODO comments inside `write_parallel.py`

Where to find us

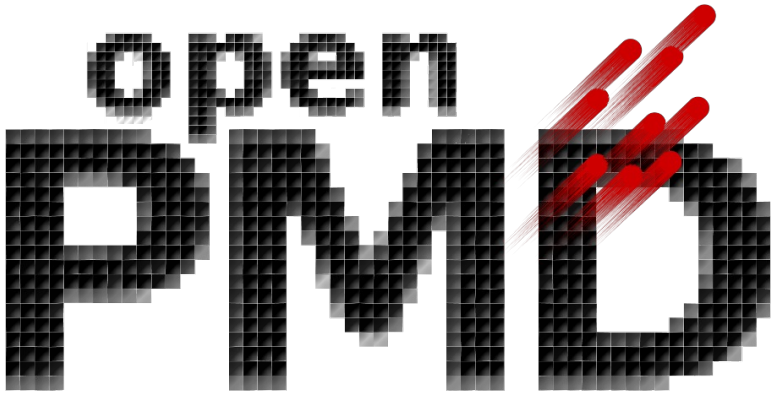
→ head to https://github.com/openPMD/



...and of course https://openpmd-api.readthedocs.io/

Community

www.openPMD.org



The **openPMD standard** is co-authored by Axel Huebl, Rémi Lehe, Jean-Luc Vay, David P. Grote, Ivo F. Sbalzarini, Stephan Kuschel, David Sagan, Frédéric Pérez, Fabian Koller, Franz Poeschel, Carsten Fortmann-Grote, Ángel Ferran Pousa, Juncheng E, Maxence Thévenet, and Michael Bussmann.

The authors are thankful for the **community contributions** to libraries, software ecosystem, user support, review and integrations. Particularly, thank you to Yaser Afshar, Lígia Diana Amorim, James Amundson, Weiming An, Igor Andriyash, Ksenia Bastrakova, Jean Luca Bez, Richard Briggs, Heiko Burau, Jong Choi, Ray Donnelly, Dmitry Ganyushin, Marco Garten, Lixin Ge, Berk Geveci, Daniel Grassinger, Alexander Grund, Junmin Gu, Marc W. Guetg, Ulrik Günther, Sören Jalas, Manuel Kirchen, John Kirkham, Scott Klasky, Noah Klemm, Fabian Koller, Mathieu Lobet, Christopher Mayes, Ritiek Malhotra, Paweł Ordyna, Richard Pausch, Norbert Podhorszki, David Pugmire, Felix Schmitt, Erik Schnetter, Dominik Stańczak, Klaus Steiniger, Michael Sippel, Frank Tsung, Lipeng Wan, René Widera, and Erik Zenker!