Efficient Management of Self-Describing Data Formats

Kira Duwe

kira.duwe@epfl.ch

May 8, 2023

DIAS

(Data-Intensive Applications and Systems Lab) École polytechnique fédérale de Lausanne (EPFL) Lausanne, Switzerland





Acknowledgments

- Work was done at
 - University of Hamburg (UHH)
 - Otto-von-Guericke University (OVGU) Magdeburg https://www.parcio.ovgu.de/
- · Thesis was supervised by Michael Kuhn
- Funded by DFG (German Research Foundation) 417705296
- More information about the CoSEMoS (Coupled Storage System for Efficient Management of Self-Describing Data Formats) project can be found at https://cosemos.de.

Outline

Motivation

Design

Evaluation

Motivation

HPC: High-Performance Computing

I/O: Input/Output

Kira Duwe

Efficient Management of Self-Describing Data Formats

Motivation

Growing data sizes

HPC: High-Performance Computing

Kira Duwe

Motivation

- Growing data sizes

Hardware hierarchy

HPC: High-Performance Computing

Motivation

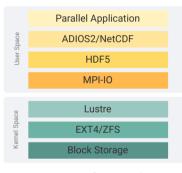
- Growing data sizes
- Hardware hierarchyLarge software stack

HPC: High-Performance Computing

I/O: Input/Output

Kira Duwe

- Growing data sizes
- Hardware hierarchy
- Large software stack

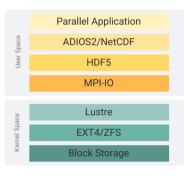


HPC I/O Software stack

HPC: High-Performance Computing

I/O: Input/Output

- Growing data sizes
- Hardware hierarchy
- Large software stack
- Optimisation for different goals

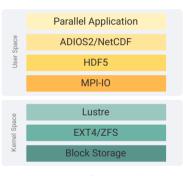


HPC I/O Software stack

HPC: High-Performance Computing

I/O: Input/Output

- Growing data sizes
- Hardware hierarchy
- Large software stack
- Optimisation for different goals
- No application changes if possible



HPC I/O Software stack

HPC: High-Performance Computing

I/O: Input/Output

I/O Libraries and their Data Formats

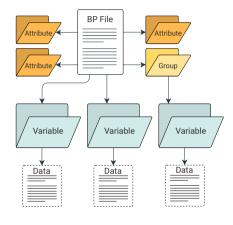
Motivation

I/O Libraries and their Data Formats

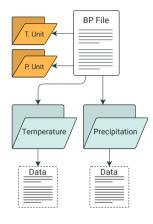
Motivation

- Common libraries: HDF5, NetCDF, ADIOS2
- Self-explanatory data through annotation
- · Ease of data sharing

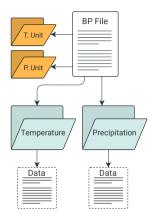
- Common libraries: HDF5, NetCDF, ADIOS2
- Self-explanatory data through annotation
- · Ease of data sharing



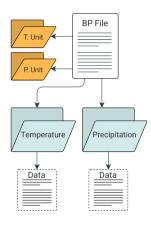
- Common libraries: HDF5, NetCDF, ADIOS2
- Self-explanatory data through annotation
- · Ease of data sharing

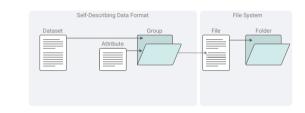


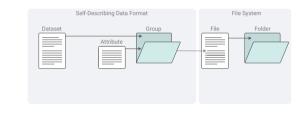
- Common libraries: HDF5, NetCDF, ADIOS2
- Self-explanatory data through annotation
- · Ease of data sharing
- Data characteristics, e.g. minima/maxima



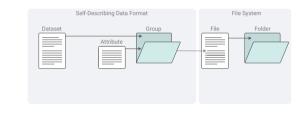
- Common libraries: HDF5, NetCDF, ADIOS2
- Self-explanatory data through annotation
- · Ease of data sharing
- Data characteristics, e.g. minima/maxima
- Block x = data written by process x



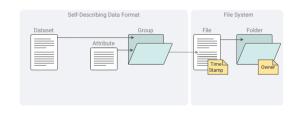




FS: file system



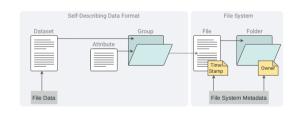
FS: file system



FS: file system

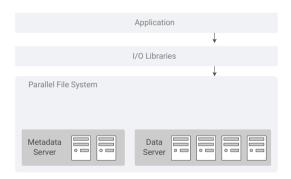


FS: file system

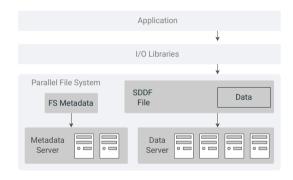


FS: file system

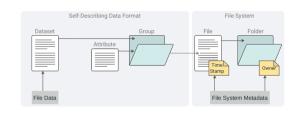
- · Currently: FS metadata and data
- · Metadata and data server



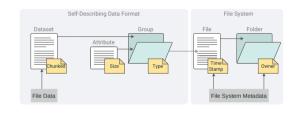
- Currently: FS metadata and data
- · Metadata and data server



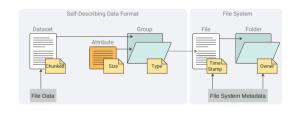
- · Currently: FS metadata and data
- · Metadata and data server
- Additional information in SDDF files



- · Currently: FS metadata and data
- · Metadata and data server
- Additional information in SDDF files

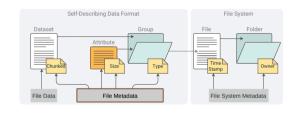


- · Currently: FS metadata and data
- · Metadata and data server
- Additional information in SDDF files



- · Currently: FS metadata and data
- · Metadata and data server
- Additional information in SDDF files

File Metadata

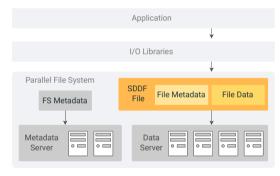


FS: file system

- · Currently: FS metadata and data
- · Metadata and data server
- Additional information in SDDF files

File Metadata

· Stored on data servers



Current Management

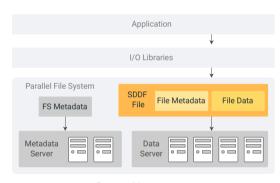
FS: file system

- · Currently: FS metadata and data
- · Metadata and data server
- · Additional information in SDDF files

File Metadata

- · Stored on data servers
- Access too limited

FS: file system



Current Management

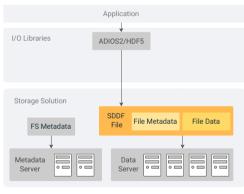
Outline

Motivation

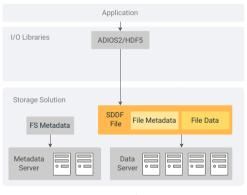
Design

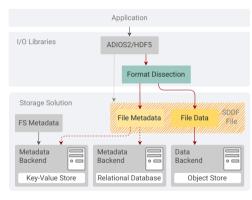
Evaluation

Design

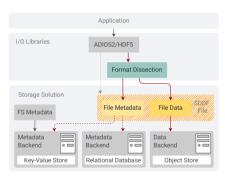


Currently



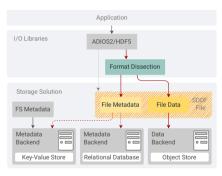


Currently Proposal



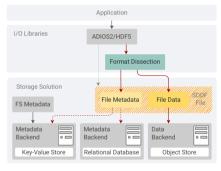
Format Dissection

→ Map file metadata to storage backends



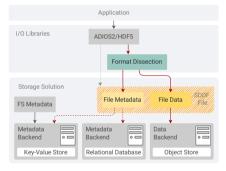
Format Dissection

- → Map file metadata to storage backends
 - Implementation in I/O library



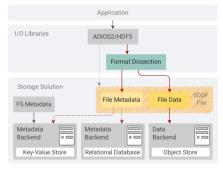
Format Dissection

- → Map file metadata to storage backends
 - Implementation in I/O library
 - Transparent to application layer



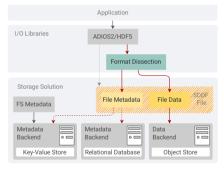
Format Dissection

- → Map file metadata to storage backends
 - Implementation in I/O library
 - Transparent to application layer
 - Using JULEA storage framework



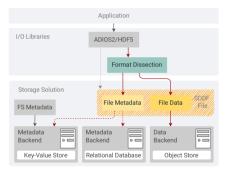
Format Dissection

- → Map file metadata to storage backends
 - Implementation in I/O library
 - Transparent to application layer
 - Using JULEA storage framework
 - 1. prototype uses key-value store



Format Dissection

- → Map file metadata to storage backends
 - Implementation in I/O library
 - Transparent to application layer
 - Using JULEA storage framework
 - 1. prototype uses key-value store
- → Demonstrate feasibility



Format Dissection

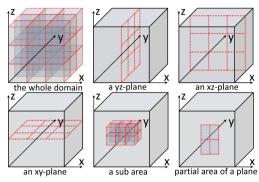
- How can metadata and data be queried efficiently?
- What custom metadata is interesting?

Design

8/16

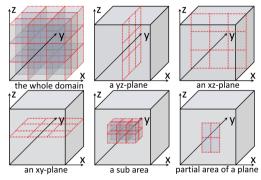
• Various patterns in literature

• Various patterns in literature



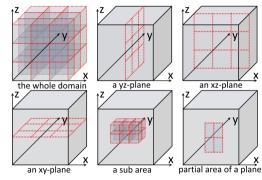
Typical access patterns [Wan et al., 2022]

- Various patterns in literature
 - \rightarrow queries not clearly defined



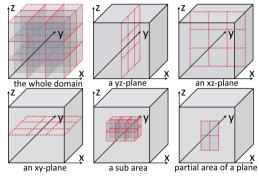
Typical access patterns [Wan et al., 2022]

- Various patterns in literature
 - → queries not clearly defined
- Data layouts can be complicated



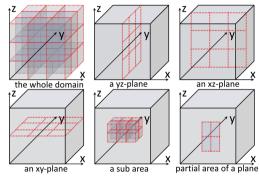
Typical access patterns [Wan et al., 2022]

- Various patterns in literature
 - → queries not clearly defined
- Data layouts can be complicated
 - → especially after dynamic load balancing



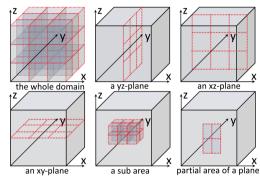
Typical access patterns [Wan et al., 2022]

- Various patterns in literature
 - → queries not clearly defined
- Data layouts can be complicated
 - \rightarrow especially after dynamic load balancing
- \rightarrow General-purpose solution required



Typical access patterns [Wan et al., 2022]

- Various patterns in literature
 - → queries not clearly defined
- Data layouts can be complicated
 - \rightarrow especially after dynamic load balancing
- ightarrow General-purpose solution required
 - 2. prototype uses a relational database



Typical access patterns [Wan et al., 2022]

^aAmong others: DKRZ, MPI, DLR, DESY, DDN, SNL, LBNL, McGill

• Researchers from different institutes ^a

^aAmong others: DKRZ, MPI, DLR, DESY, DDN, SNL, LBNL, McGill

- Researchers from different institutes ^a
- 22 completed, 38 in total

^aAmong others: DKRZ, MPI, DLR, DESY, DDN, SNL, LBNL, McGill

- Researchers from different institutes ^a
- 22 completed, 38 in total

• 1. Format usage

- Researchers from different institutes ^a
- 22 completed, 38 in total
- 1. Format usage
- ightarrow Informed database schema design

 $[^]a$ Among others: DKRZ, MPI, DLR, DESY, DDN, SNL, LBNL, McGill

Design

- Researchers from different institutes ^a
- 22 completed, 38 in total
- 1. Format usage
- → Informed database schema design
- 2. Post-processing

 $^a\mathrm{Among}$ others: DKRZ, MPI, DLR, DESY, DDN, SNL, LBNL, McGill

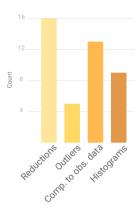
Design

- Researchers from different institutes ^a
- 22 completed, 38 in total
- 1. Format usage
 - → Informed database schema design
- 2. Post-processing
 - → Guided custom metadata choice

 $^a\mathrm{Among}$ others: DKRZ, MPI, DLR, DESY, DDN, SNL, LBNL, McGill

User Survey Design

- Researchers from different institutes ^a
- 22 completed, 38 in total
- 1. Format usage
 - → Informed database schema design
- 2. Post-processing
 - → Guided custom metadata choice



Typical post-processing operations

^aAmong others: DKRZ, MPI, DLR, DESY, DDN, SNL, LBNL, McGill

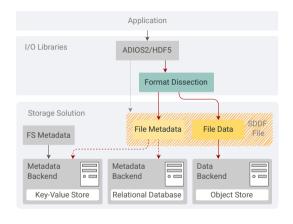
- Precompute common post-processing operations (default: mean and sum)
 - → Reduce data access for analysis

- Precompute common post-processing operations (default: mean and sum)
 - → Reduce data access for analysis
- · Tagging functionality
 - → *Mark interesting data parts*

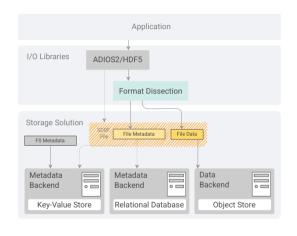
- Precompute common post-processing operations (default: mean and sum)
 - → Reduce data access for analysis
- · Tagging functionality
 - → *Mark interesting data parts*
- Read
 - \rightarrow Enable querying

- Precompute common post-processing operations (default: mean and sum)
 - → Reduce data access for analysis
- · Tagging functionality
 - → *Mark interesting data parts*
- Read
 - \rightarrow Enable querying

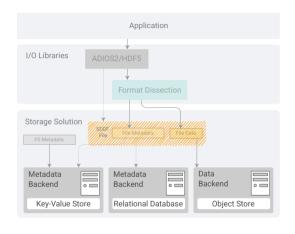
- Precompute common post-processing operations (default: mean and sum)
 - → Reduce data access for analysis
- Tagging functionality
 - → Mark interesting data parts
- Read
 - → Enable querying



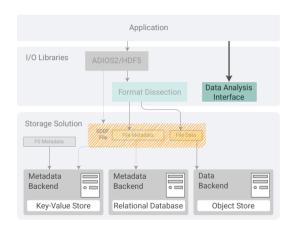
- Precompute common post-processing operations (default: mean and sum)
 - → Reduce data access for analysis
- Tagging functionality
 - → *Mark interesting data parts*
- Read
 - → Enable querying



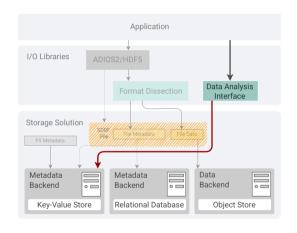
- Precompute common post-processing operations (default: mean and sum)
 - → Reduce data access for analysis
- Tagging functionality
 - → *Mark interesting data parts*
- Read
 - → Enable querying



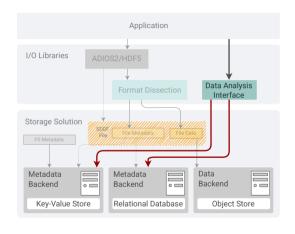
- Precompute common post-processing operations (default: mean and sum)
 - → Reduce data access for analysis
- Tagging functionality
 - → Mark interesting data parts
- Read
 - → Enable querying



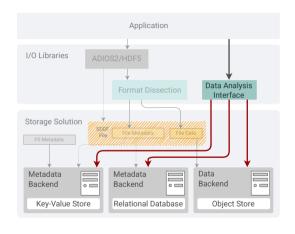
- Precompute common post-processing operations (default: mean and sum)
 - → Reduce data access for analysis
- Tagging functionality
 - → *Mark interesting data parts*
- Read
 - → Enable querying



- Precompute common post-processing operations (default: mean and sum)
 - → Reduce data access for analysis
- Tagging functionality
 - → *Mark interesting data parts*
- Read
 - → Enable querying



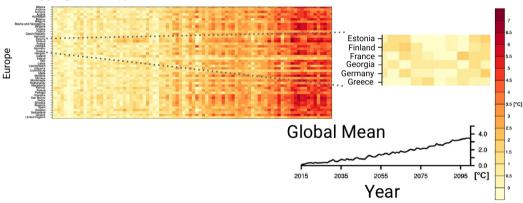
- Precompute common post-processing operations (default: mean and sum)
 - → Reduce data access for analysis
- Tagging functionality
 - → *Mark interesting data parts*
- Read
 - → Enable querying



• Aggregations typical for climate research

• Aggregations typical for climate research

Aggregations typical for climate research

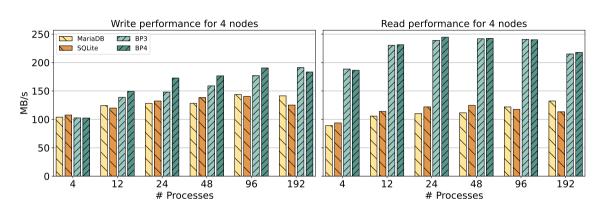


Outline

Motivation

Design

Evaluation



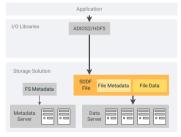
published at SYSTOR 2021

Evaluation

• Examine performance for different queries

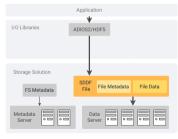
- Examine performance for different queries
- Comparing different I/O paths

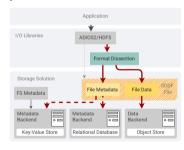
- Examine performance for different queries
- Comparing different I/O paths



BP

- Examine performance for different queries
- Comparing different I/O paths

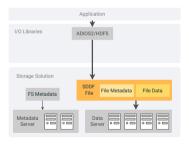


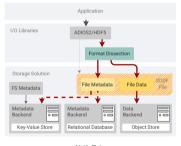


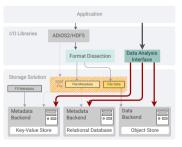
BP

JULEA

- Examine performance for different queries
- Comparing different I/O paths







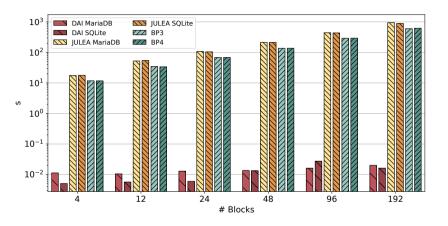
BP

JULEA

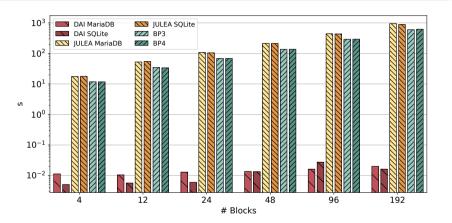
DAI

Evaluation

 $\,\rightarrow\,$ Retrieve largest difference between block mean value in step 1 and 5

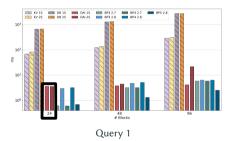


ightarrow Retrieve largest difference between block mean value in step 1 and 5

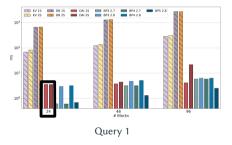


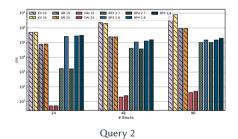
- → Retrieve largest difference between block mean value in step 1 and 5
 - For 192 blocks: 0.01 s (DAI) and 621/601 s (BP3/BP4)

No one size fits all

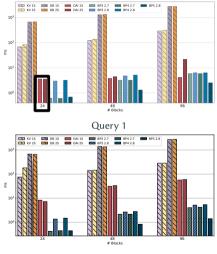


No one size fits all Evaluation



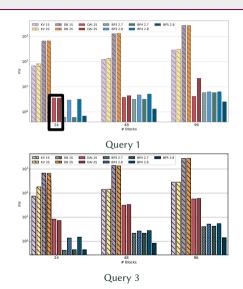


No one size fits all Evaluation



Query 3

No one size fits all



Query 2 و 10⁴

Blocks

Query 4

Generalising the Approach

Evaluation

Generalising the Approach

Evaluation

• Works for more than one format [Kuhn and Duwe, CSCI 2020]

- Works for more than one format [Kuhn and Duwe, CSCI 2020]
- Applicable to different scientific fields

- Works for more than one format [Kuhn and Duwe, CSCI 2020]
- Applicable to different scientific fields
- Problem: data models differ, e.g.

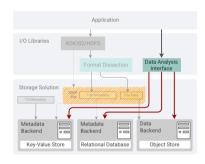
- Works for more than one format [Kuhn and Duwe, CSCI 2020]
- · Applicable to different scientific fields
- · Problem: data models differ, e.g.
 - · All data in a single 4D dataset

- Works for more than one format [Kuhn and Duwe, CSCI 2020]
- · Applicable to different scientific fields
- Problem: data models differ, e.g.
 - All data in a single 4D dataset
 - A separate 3D dataset for each step

- Works for more than one format [Kuhn and Duwe, CSCI 2020]
- Applicable to different scientific fields
- Problem: data models differ, e.g.
 - All data in a single 4D dataset
 - A separate 3D dataset for each step
 - A separate file for each step

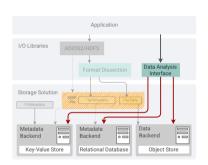
- Works for more than one format [Kuhn and Duwe, CSCI 2020]
- · Applicable to different scientific fields
- Problem: data models differ, e.g.
 - · All data in a single 4D dataset
 - A separate 3D dataset for each step
 - · A separate file for each step
 - → Either significant abstractions or restrictive modelling

- Works for more than one format [Kuhn and Duwe, CSCI 2020]
- · Applicable to different scientific fields
- Problem: data models differ, e.g.
 - · All data in a single 4D dataset
 - A separate 3D dataset for each step
 - · A separate file for each step
 - → Either significant abstractions or restrictive modelling
- Implementation for every library \rightarrow not easily scalable

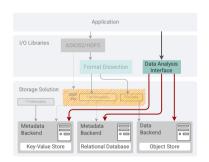


Conclusion

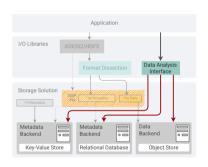
• Dissecting formats enables new management options



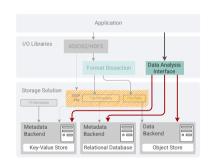
- Dissecting formats enables new management options
- · No changes in simulation codes required



- Dissecting formats enables new management options
- · No changes in simulation codes required
- Pre-computation of statistics can be very beneficial



- Dissecting formats enables new management options
- · No changes in simulation codes required
- Pre-computation of statistics can be very beneficial
- DAI can achieve impressive performance (60,000 x)



Bibliography

- [Duwe and Kuhn, 2021a] Duwe, K. and Kuhn, M. (2021a). Dissecting Self-Describing Data

 Formats to Enable Advanced Querying of File Metadata. In Proceedings of the 14th ACM

 International Conference on Systems and Storage, SYSTOR '21, New York, NY, USA.

 Association for Computing Machinery.
- [Duwe and Kuhn, 2021b] Duwe, K. and Kuhn, M. (2021b). Using Ceph's BlueStore as Object Storage in HPC Storage Framework. In Proceedings of the Workshop on Challenges and Opportunities of Efficient and Performant Storage Systems, CHEOPS '21, New York, NY, USA. Association for Computing Machinery.
- [Duwe et al., 2020] Duwe, K., Lüttgau, J., Mania, G., Squar, J., Fuchs, A., Kuhn, M., Betke, E., and Ludwig, T. (2020). State of the Art and Future Trends in Data Reduction for High-Performance Computing. Supercomput. Front. Innov., 7(1):4–36.

Bibliography ...

- [Kuhn and Duwe, 2020] Kuhn, M. and Duwe, K. (2020). Coupling Storage Systems and Self-Describing Data Formats for Global Metadata Management. In 2020 International Conference on Computational Science and Computational Intelligence (CSCI), pages 1224–1230.
- [Lüttgau et al., 2018] Lüttgau, J., Kuhn, M., Duwe, K., Alforov, Y., Betke, E., Kunkel, J. M., and Ludwig, T. (2018). **Survey of Storage Systems for High-Performance Computing.** Supercomput. Front. Innov., 5(1):31–58.
- [Wan et al., 2022] Wan, L., Huebl, A., Gu, J., Poeschel, F., Gainaru, A., Wang, R., Chen, J., Liang, X., Ganyushin, D., Munson, T. S., Foster, I. T., Vay, J., Podhorszki, N., Wu, K., and Klasky, S. (2022). Improving I/O performance for exascale applications through online data layout reorganization. IEEE Trans. Parallel Distributed Syst., 33(4):878–890.