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EMPRESS—Extensible Metadata PRovider for Extreme-scale Scientific Simulations

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Problems Faced

- Simulations with 100s TB per output, run every few minutes
  - Ex. XGC1, Square Kilometer Array Radio Telescope (SKA)

- Storage devices too slow to sift through all output to find “interesting data”

- Scientists have specific data they want to retrieve
  - Ex. “blob” in fusion reactor or a phenomenon in astronomy

Motivating Question

How can we facilitate scientific discovery from simulations in the exascale age?

EMPRESS’ Solution

- Allow users to label data and retrieve data based on labels

- Features:
  - Robust, standard per-process metadata
  - User-created metadata that is fully customizable at runtime
  - Programmatic query API to retrieve data contents based on metadata

Previous Solutions

- HDF5 and NetCDF – rudimentary attribute capabilities, basic metadata
- ADIOS – per-process metadata

None of these address efficient attribute searching

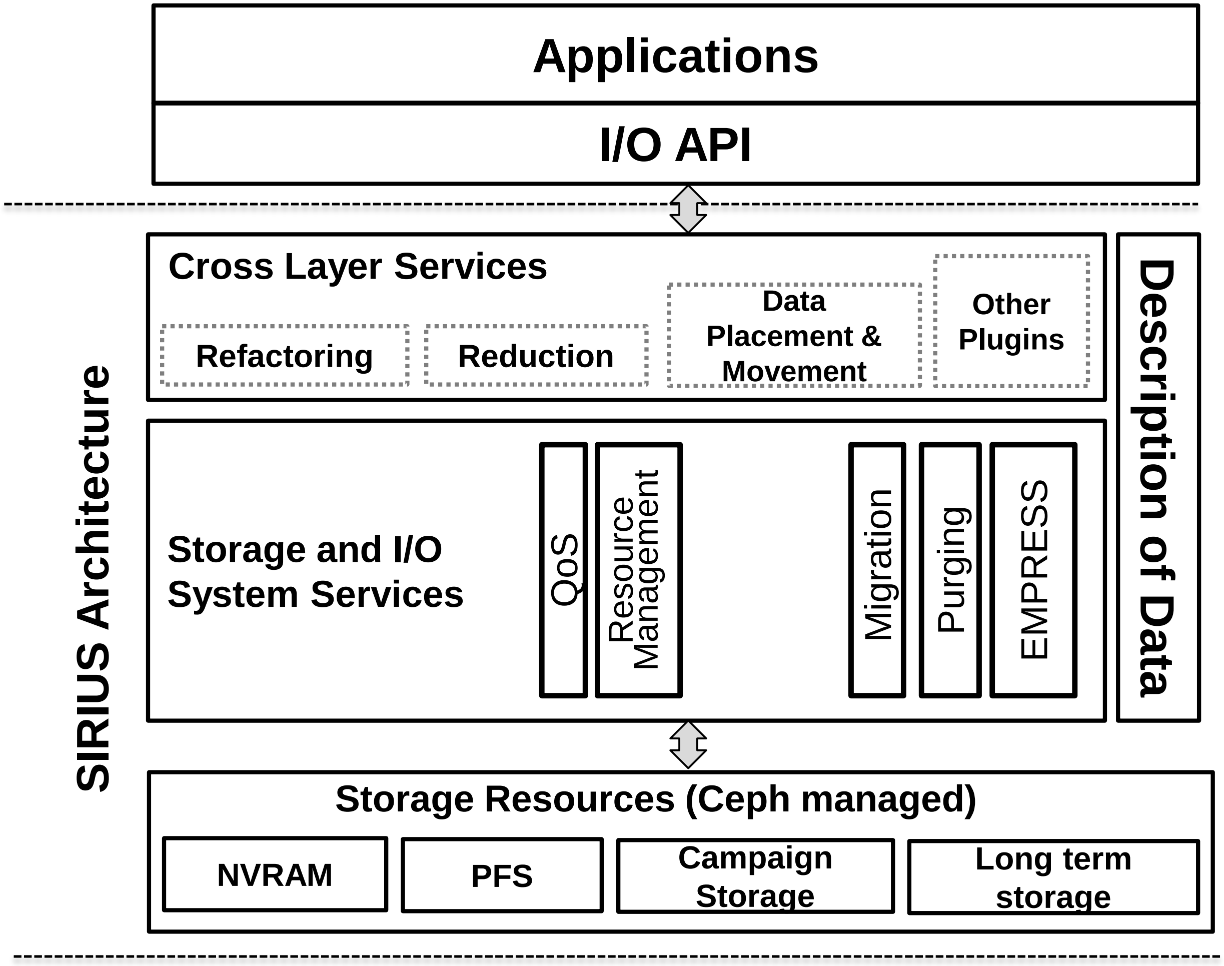
- FastBit – offers data querying based on values, but very limited support for spatial queries and attributes

Why not use a Key-Value Store?

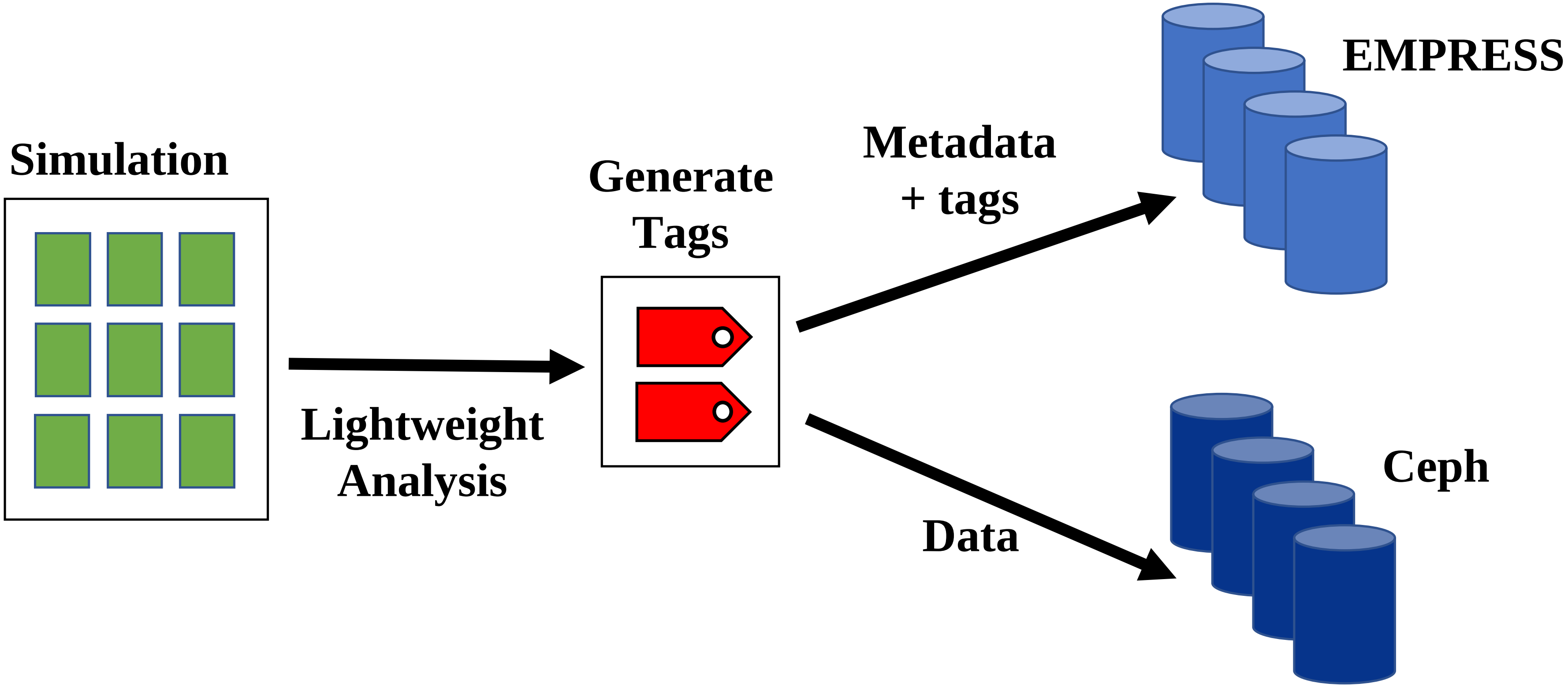
- Custom keys can go a long way, but not far enough
- Two Problems:
  - Inexact matches
  - Custom Metadata

- Relational databases with indices are radically faster at searching like this

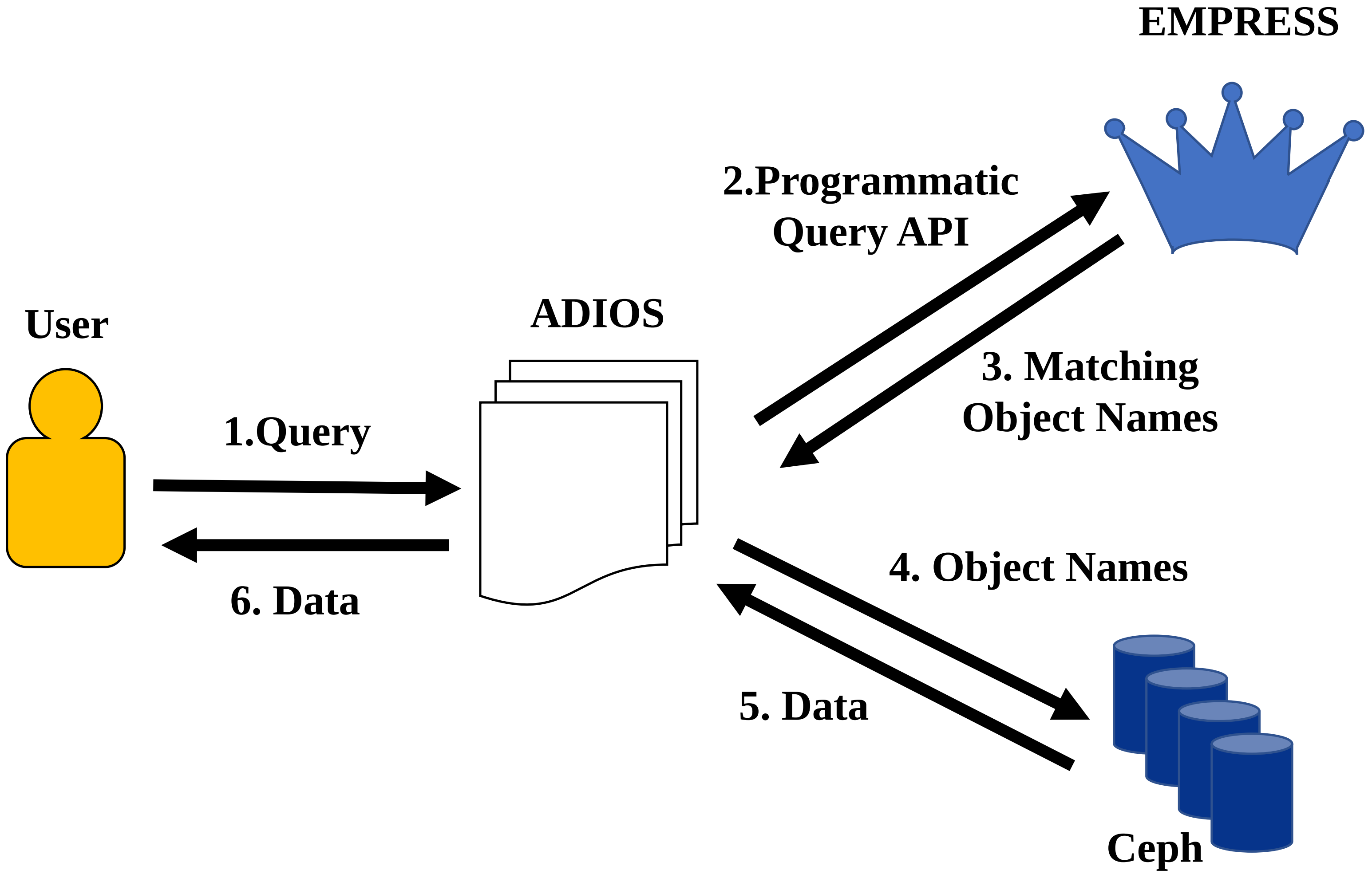
SIRIUS Architecture



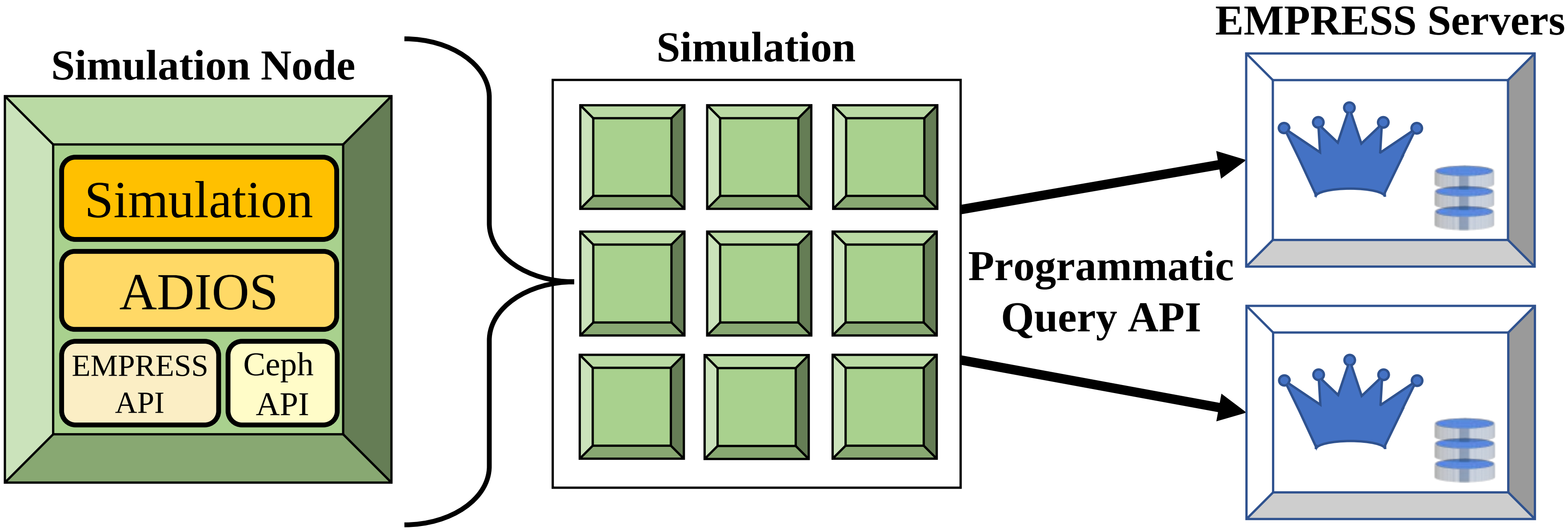
SIRIUS Workflow – Write Process



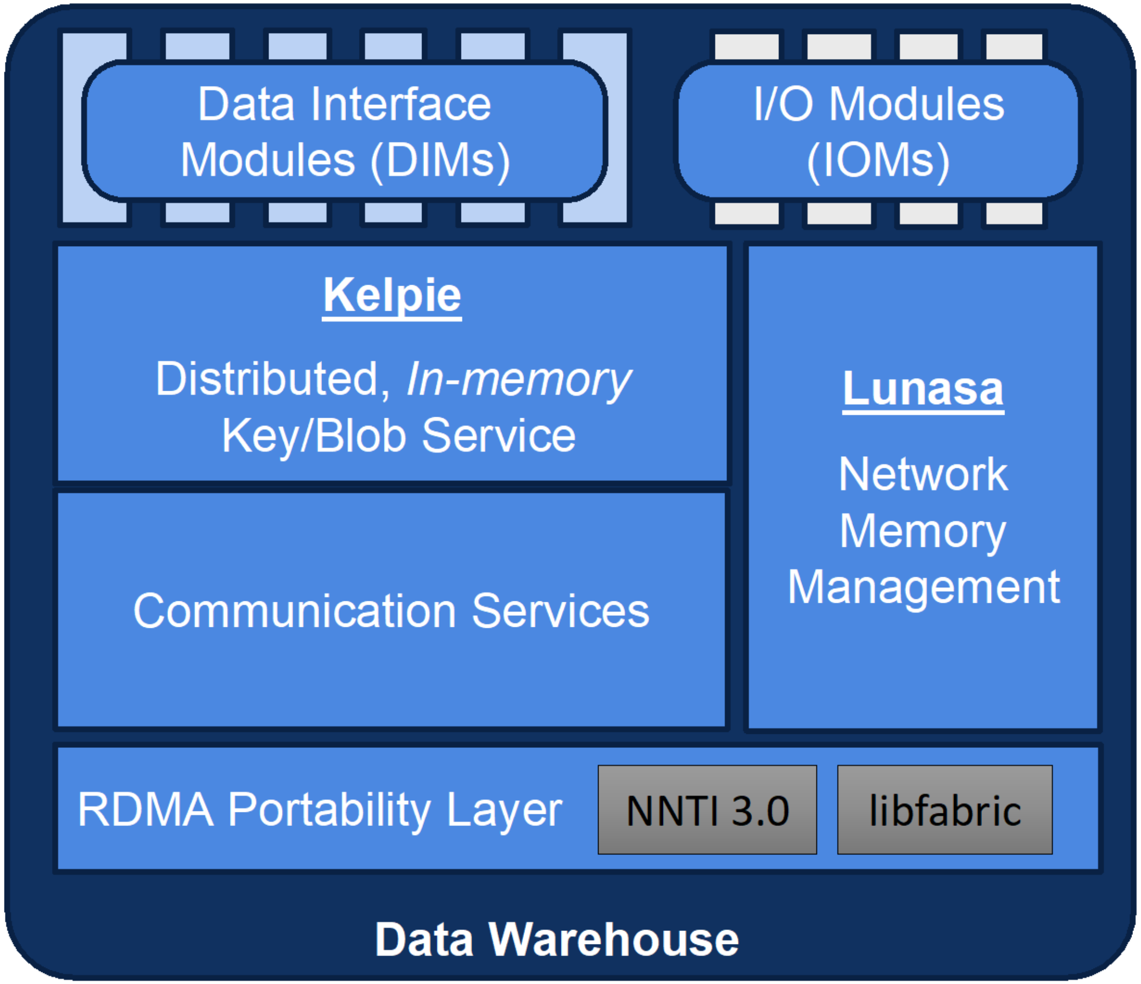
SIRIUS Workflow – Read Process



High Level Design



Faodail



Data Interface Modules (DIMs)
I/O Modules (IOMs)
Kelpie
Distributed, *In-memory* Key/Blob Service
Lunasa
Network Memory Management
Communication Services
RDMA Portability Layer
NNTI 3.0
libfabric
Data Warehouse

Storage - Tracked Metadata

- Dataset information
  - Application, run, and timestep information
- Variable information
  - Catalogs types of data stored for an output operation
- Variable chunk information
  - Subdivision of simulation space associated with a particular variable
- Custom metadata class
  - Metadata category the user adds for a particular dataset
  - Ex. Max
- Custom metadata instance
  - Ex. Flag for chunk or a bounding box spanning chunks

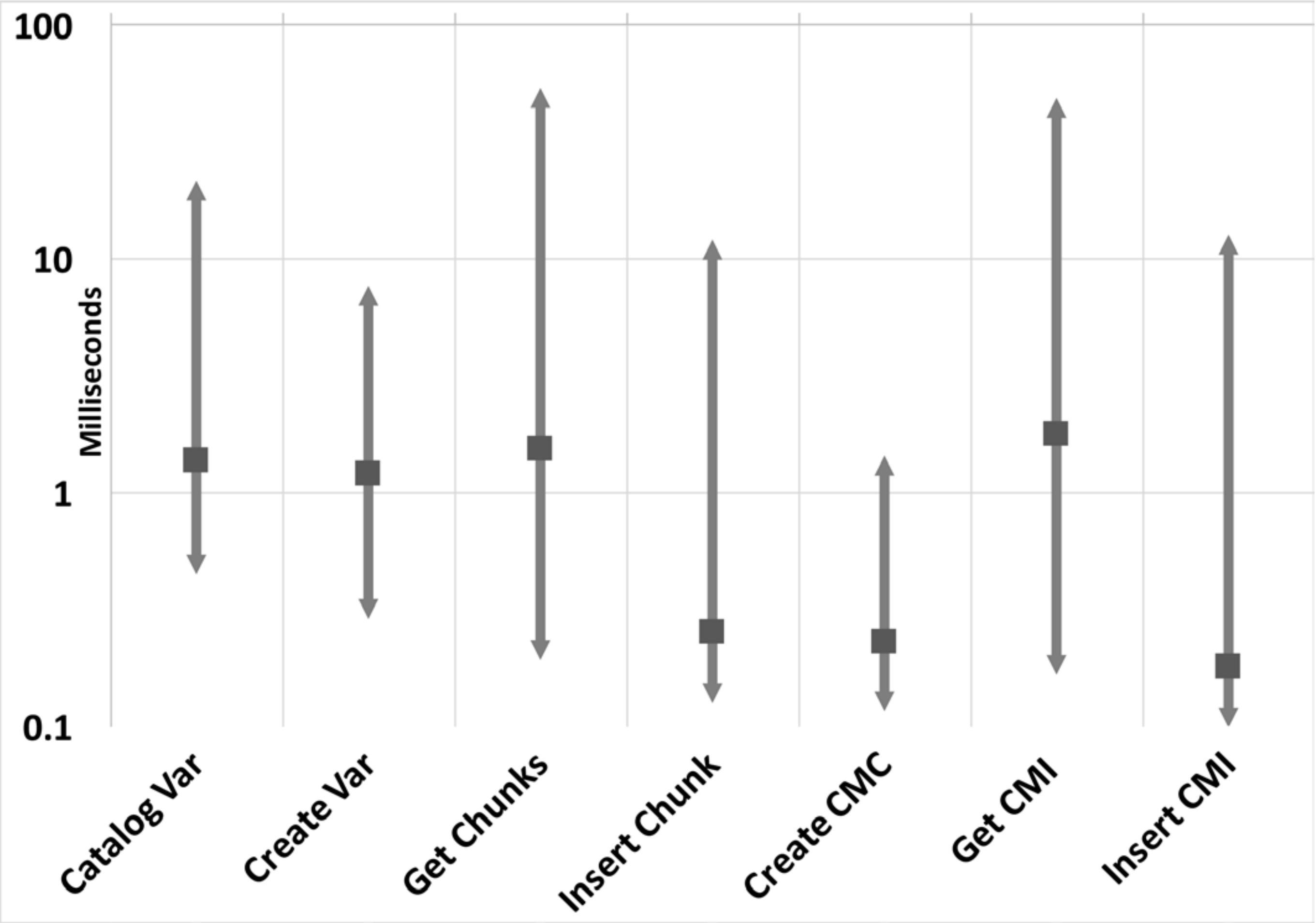
Testing Goals

- Scalable?
  - Number of client processes: 1024-2048
- Effect of client to server ratio
  - Ratios tested: 32:1 – 128:1
- Overhead of including a large number of custom metadata items
  - Number of custom metadata classes: 0 or 10
  - On average 2.641 custom metadata instances per chunk

Testing Goals (Continued)

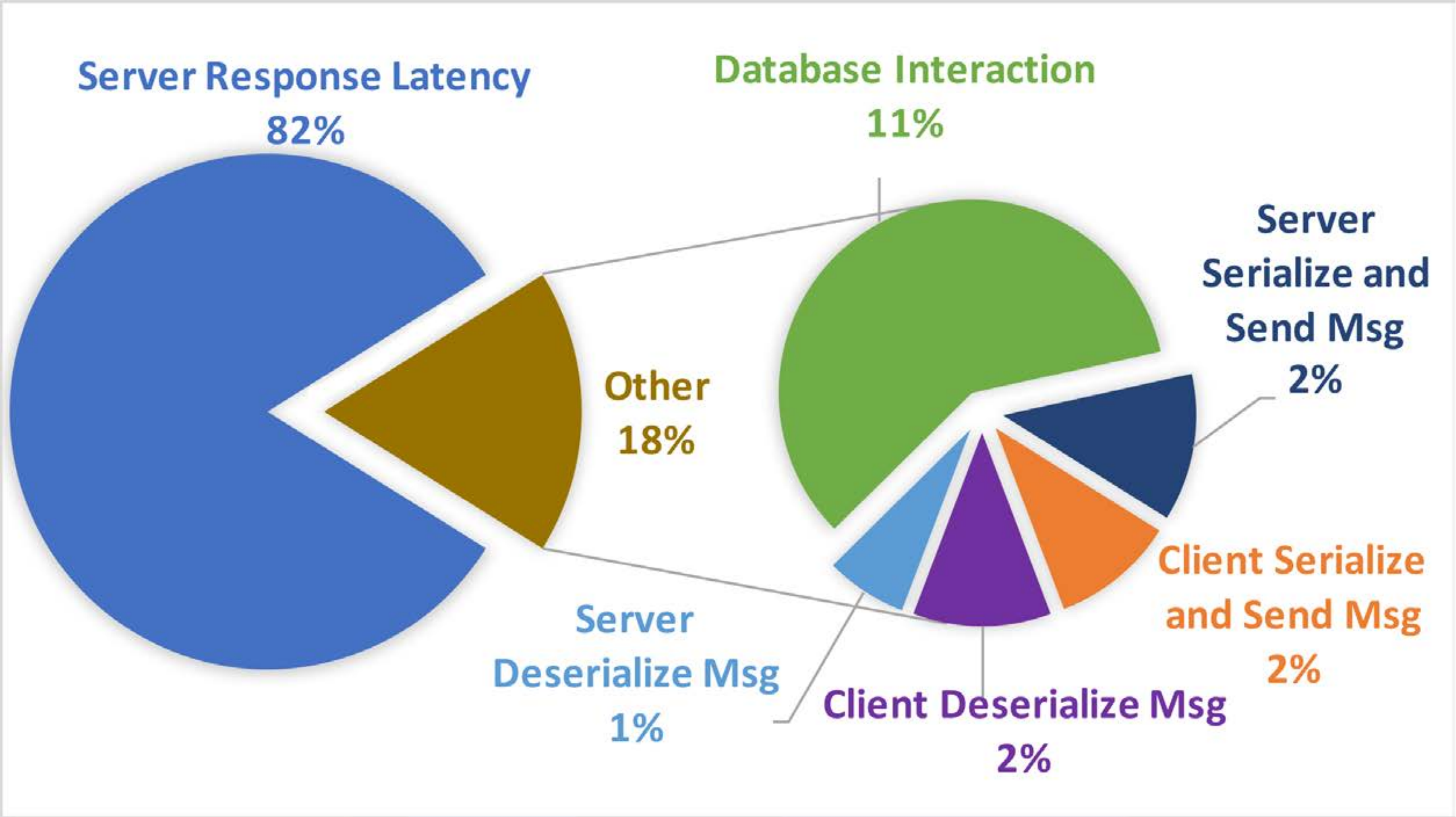
- Proof of concept, can EMPRESS efficiently support:
  - Common writing operations
    - 2 datasets written, each with 10 globally distributed 3-D arrays
  - Common reading operations
    - 6 different read patterns that scientists frequently use (Lofstead, et al. "Six Degrees of Scientific Data")
  - A broad range of custom metadata
    - 10 custom metadata classes including max, flag, bounding box (two 3-D points)
- Scientific validity
  - A minimum of 5 runs per configuration on 3 computing clusters:
    - Serrano (total nodes: 1122)
    - Skybridge (total nodes: 1848)
    - Chama (total nodes: 1232)

Testing – Query Times



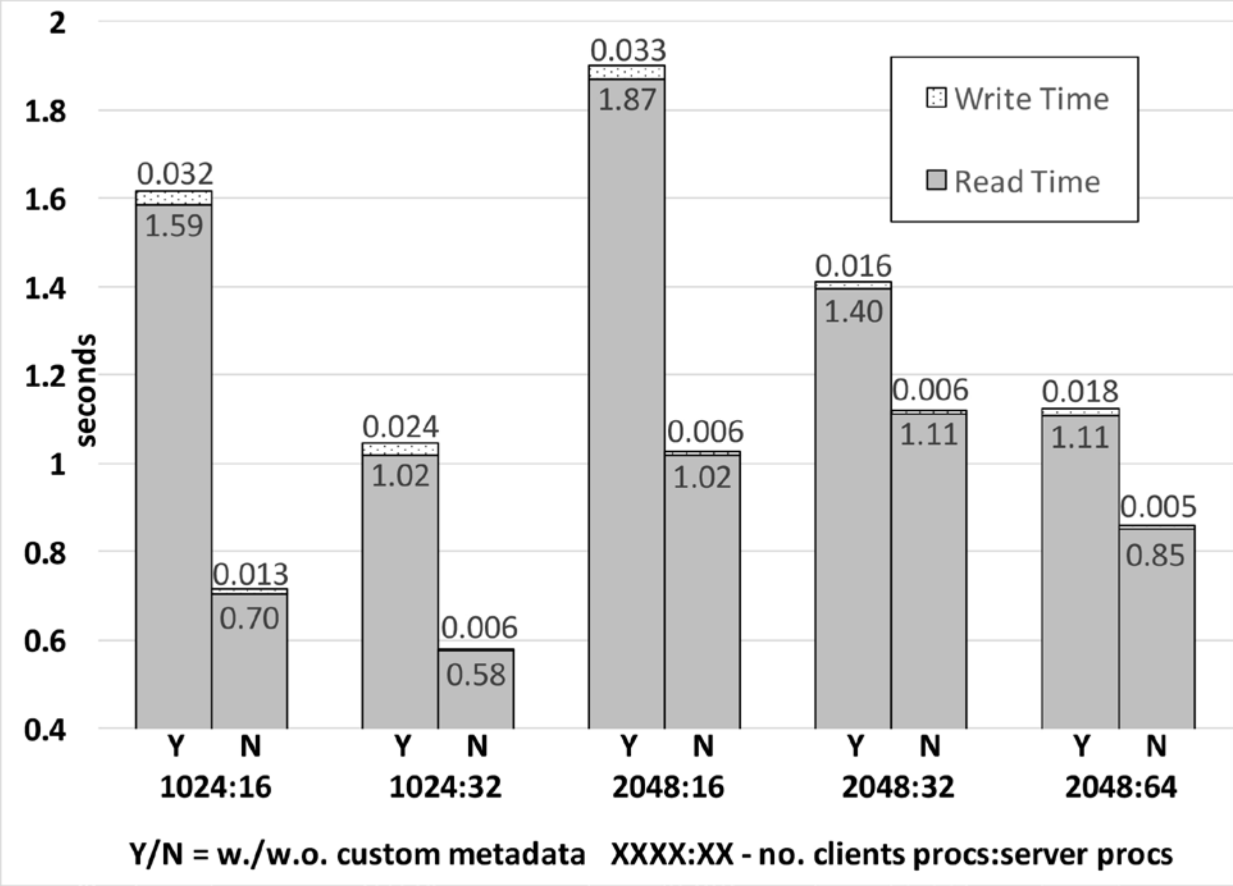
- EMPRESS efficiently supports a wide variety of operations including custom metadata operations

Testing – Chunk Retrieval Time



- Most time is spent waiting for the server to respond
  - Room for improvement in the Faodail infrastructure

Testing – Writing and Reading Time



- Good scalability for fixed client-server ratio
- No significant overhead for adding custom metadata
- Client-server ratio greatly affects performance

Future Work

- Increasing EMPRESS’ flexibility, efficiency, and scalability
  - Support more queries
  - Different metadata distribution?

Acknowledgements

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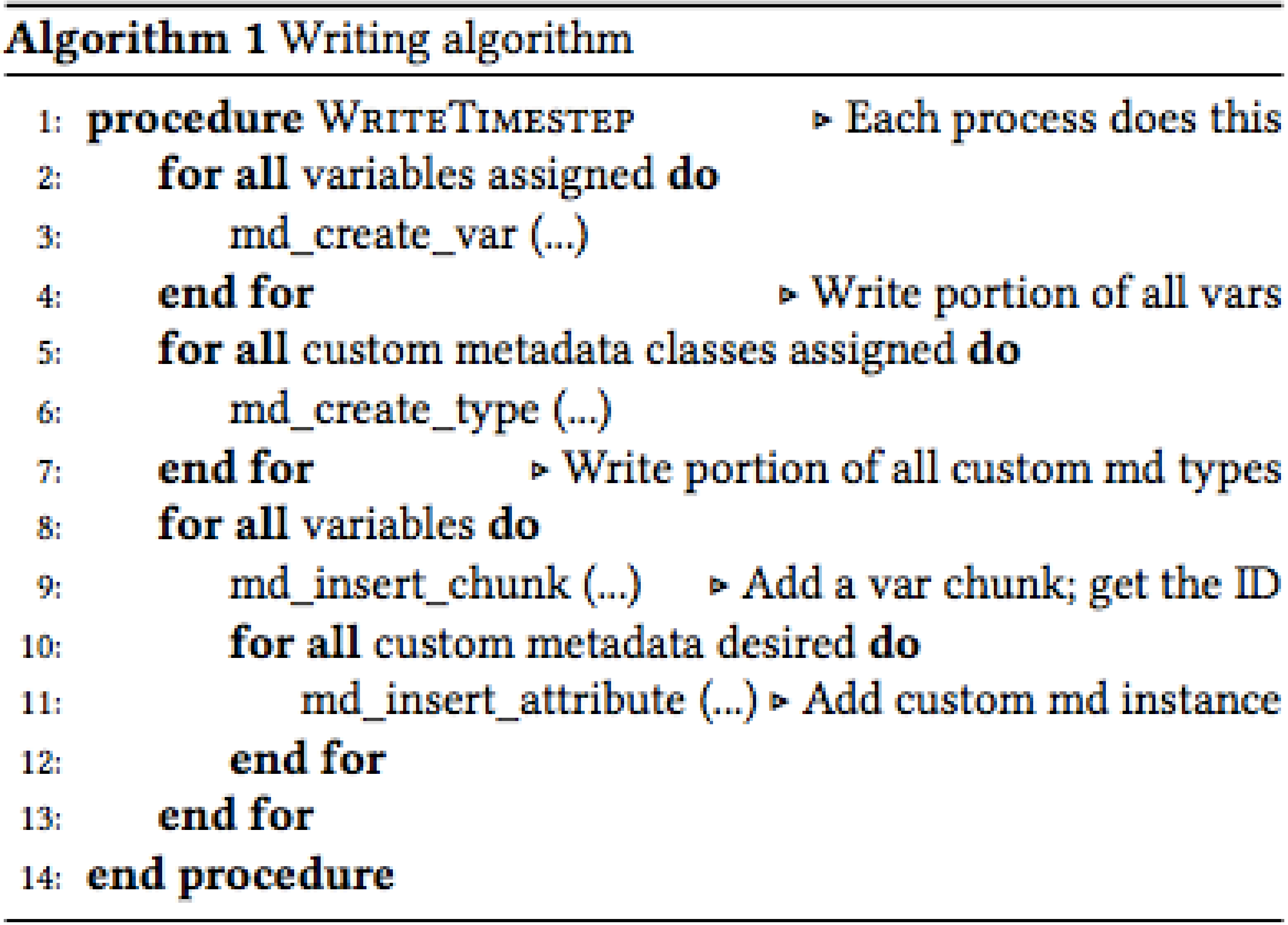
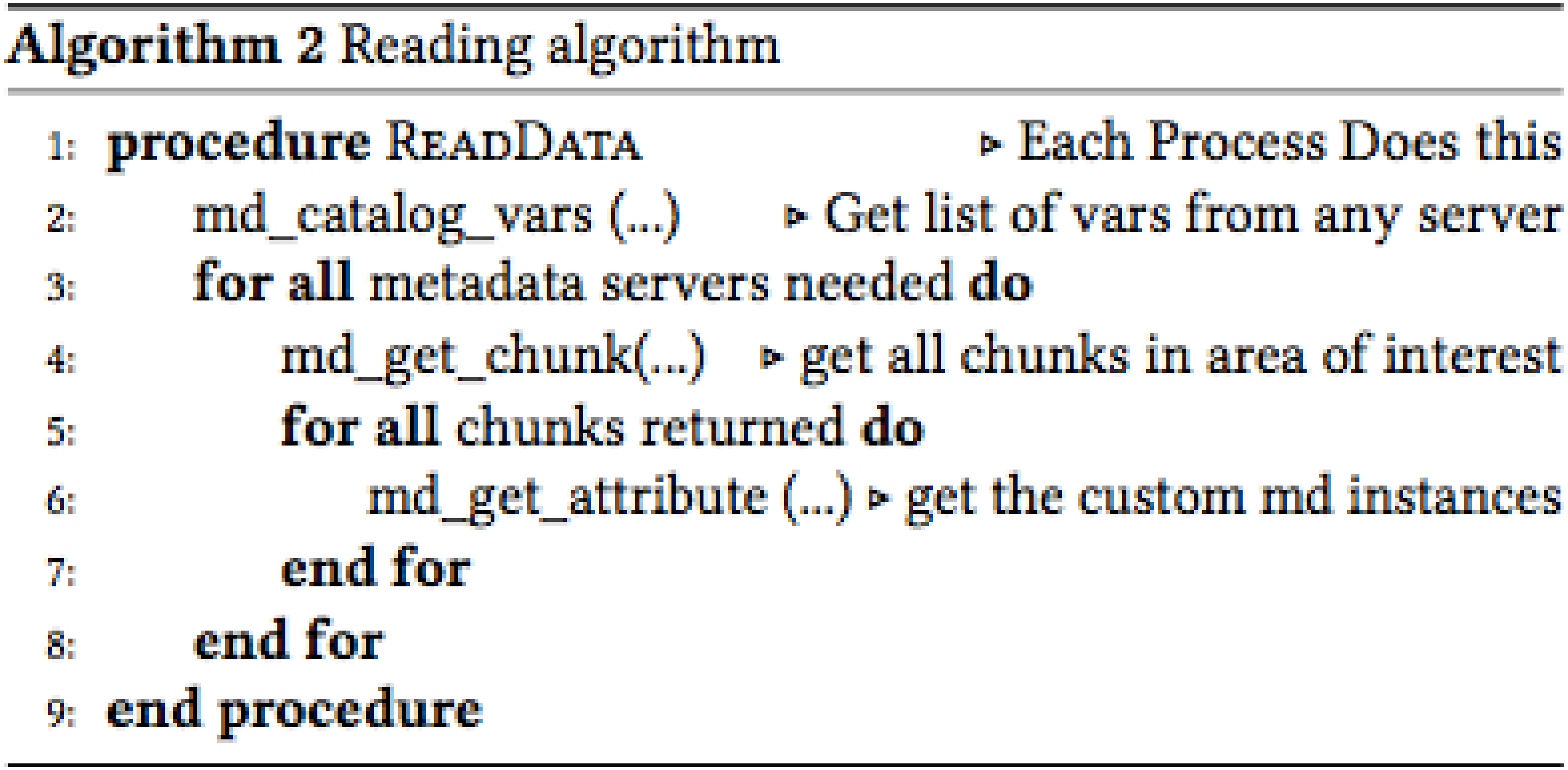


Algorithm 1 Writing algorithm

```
procedure WriteTimestep                                  ▷ Each process does this
    for all variables assigned do
        md_create_var (...)
    end for                                              ▷ Write portion of all vars
    for all custom metadata classes assigned do
        md_create_type (...)
    end for                                ▷ Write portion of all custom md types
    for all variables do
        md_insert_chunk (...)                       ▷ Add a var chunk; get the ID
        for all custom metadata desired do
            md_insert_attribute (...)               ▷ Add custom md instance
        end for
    end for
end procedure
```



Algorithm 2 Reading algorithm

```
procedure ReadData                                        ▷ Each Process Does this
    md_catalog_vars (...)                  ▷ Get list of vars from any server
    for all metadata servers needed do
        md_get_chunk(...)             ▷ get all chunks in area of interest
        for all chunks returned do
            md_get_attribute (...) ▷ get the custom md instances
        end for
    end for
end procedure
```