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Using a Robust Metadata Management System to Accelerate Scientific Discovery at Extreme Scales

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Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.



Problems Faced



- A single output can produce a dataset in the terabyte to petabyte range
- Large datasets are very slow to move and search
- Scientists have limited allocations of computational resources

Custom Metadata Solution





Previous Work - EMPRESS 1.0



- Proof of concept
 - Rich, custom metadata management can be supported with reasonable efficiency and scalability
- Next steps
 - Improving the efficiency, scalability, and functionality to create a viable production system

Paper Contributions



- EMPRESS 2.0
 - Queries
 - Atomic operations
 - Fault tolerance
 - Portability
- RDBMS is a viable HPC technology for data-oriented metadata

Metadata Model





Custom Metadata Queries



- Supports a wide variety of queries including global, spatial, temporal and multivariate
 - E.g., list all runs or timesteps that contain a "blob" near the reactor edge

Atomic Operations



- Low overhead transactions
 - Transactions are atomic (committed in their entirety or aborted)
 - Metadata is given a transaction id that determines its external visibility
 - Eliminates the need for locks or blocking of service
 - The implementation is largely based on the D²T system^[1]

Fault Tolerance



- Users can choose how to recover from failures occurring at the function, transaction, and hardware levels
- Basic metadata may be redundant, preventing data loss
 - E.g., if used with an I/O system

Portability



- Directly storing the names of associated data objects limits portability and scalability
- EMPRESS 2.0 does not store the names, it uses a function to generate them
 - All EMPRESS metadata is portable

Implementation





Evaluation - Experiment Types



Test Type	# Write	# Read	# Metadata
lest type	Procs	Procs	Servers
EMPRESS 2.0 + HDF5	1000	100	1
EMPRESS 2.0 + HDF5	2000	200	2
EMPRESS 2.0 + HDF5	4000	400	4
HDF5	1000	100	N/A
HDF5	2000	200	N/A
HDF5	4000	400	N/A

Evaluation – Write Process



- Run structure:
 - One application run, three timesteps, ten 3-D variables
- Data
 - Each process writes 0.4GB of data (10% of RAM) per timestep
- Custom metadata:
 - 10 different tags of varying frequency
 - On average, each process writes 26 attributes per timestep (2.6 per variable)

Evaluation – Read Process



- 1. 6 common read patterns^[2] are performed including
 - 1. An entire variable
 - 2. A plane and partial plane in each dimension
 - 3. A 3-D subspace
- 2. Custom metadata is used to identify potential features of interest and the associated data is read in

Evaluation – Writing



# Write	Data	EMPR Md	EMPR Md	HDF5 Md	HDF5 Md
Procs	Write	Write	Overhead	Write	Overhead
1000	1753s	1.53 s	0.09%	0.66s	0.04%
2000	3852s	1.65s	0.04%	1.80 s	0.05%
4000	7406s	1.56 s	0.02%	3.22s	0.04%

- Both can do efficient metadata writes at the evaluated scales
 - But EMPRESS can scale out to achieve constant performance

Evaluation – Metadata Read





 HDF5 takes almost as long to do the metadata query as it does to read the data

Evaluation – Accelerating Data Reads

Single Variable Read Time Vs. Selectivity



 EMPRESS can significantly accelerate data reads by limiting the scope to data of interest

Future Work - EMPRESS



- Evaluation
 - Potential bottlenecks & solutions
 - Comparison to more alternatives
 - NoSQL vs RDBMS
- Functionality
 - Expanding the application classes that EMPRESS can support

Conclusions



- Custom metadata is an important tool for accelerating post-processing
- Current I/O tools cannot efficiently support custom metadata services
- EMPRESS 2.0 offers insights on the functionalities needed for a production system & how to implement them scalably

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Citations



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