SDS: A Framework for Scientific Data Services

Bin Dong, Suren Byna*, John Wu

Scientific Data Management Group

Lawrence Berkeley National Laboratory

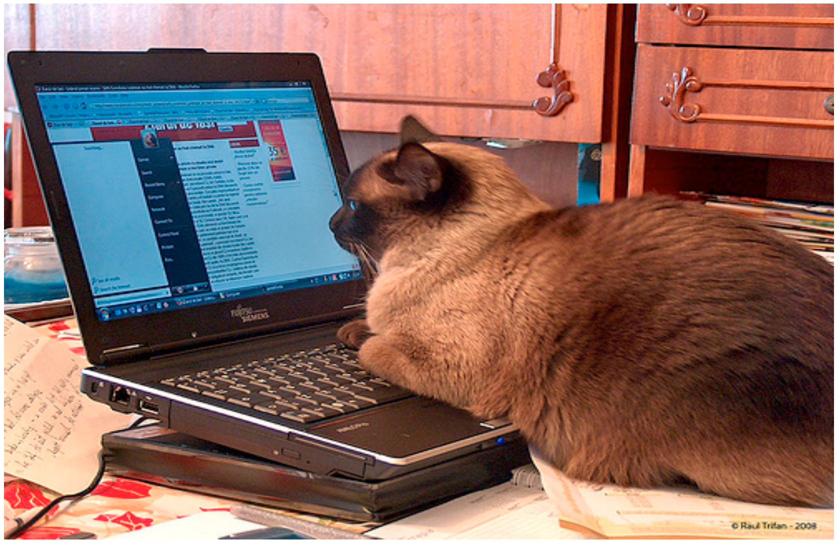
Finding Newspaper Articles of Interest

- **Finding news articles of your interest in the old era of print newspaper**
  - Turn pages
  - Read headlines
  - Searching for specific news was time consuming
- **Online newspapers**
  - Search box
  - Limited to one newspaper
- **Customized News**
  - Articles are organized based on reader's interest
  - Search numerous online newspapers


Chicago Sunday Tribune
FINAL EDITION
JURY CONVICTS CAPONE
omas A. Edison Dies in Sleep at 84
Kill Matt Kolb, Northwest Side Gambling Czar
GANG MONARCH GUILTY ON 5 TAX FRAUD COUNTS
Faces Possibility of 17 Years in Cell.
DEATH PAINLESS FOR MAN WHO LIGHTED WORLD
Family at Bedside When End Comes.
INJUN SUMMER
SUMMARY

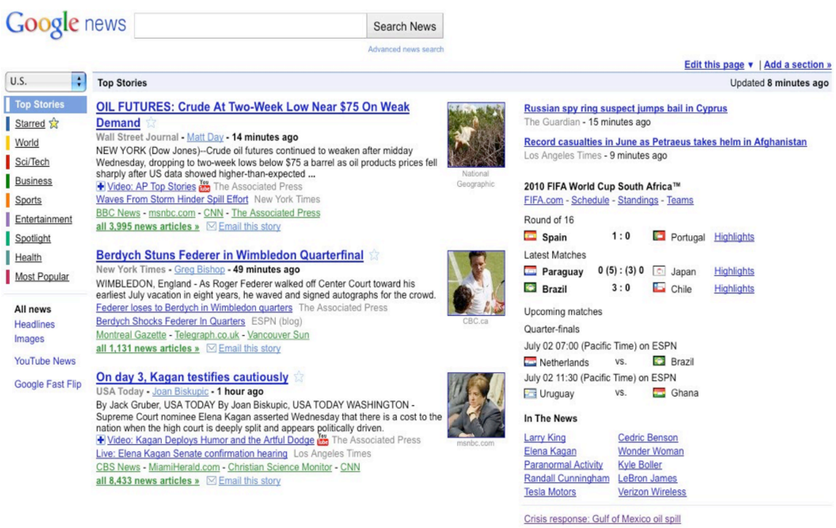
Finding Newspaper Articles of Interest

- **Finding news articles of your interest in the old era of print newspaper**
  - Turn pages
  - Read headlines
  - Searching for specific news was time consuming
- **Online newspapers**
  - Search box
  - Limited to one newspaper
- **Customized News**
  - Articles are organized based on reader's interest
  - Search numerous online newspapers



Finding Newspaper Articles of Interest

- **Finding news articles of your interest in the old era of print newspaper**
  - Turn pages
  - Read headlines
  - Searching for specific news was time consuming
- **Online newspapers**
  - Search box
  - Limited to one newspaper
- **Customized News**
  - Articles are organized based on reader's interest
  - Search numerous online newspapers



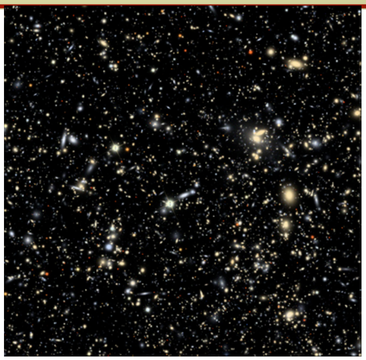
Finding Newspaper Articles of Interest

- **Finding news articles of your interest in the old era of print newspaper**
  - Turn pages
  - Read headlines
  - Searching for specific news was time consuming
- **Online newspapers**
  - Search box
  - Limited to one newspaper
- **Customized News**
  - Articles are organized based on reader's interest
  - Search numerous online newspapers

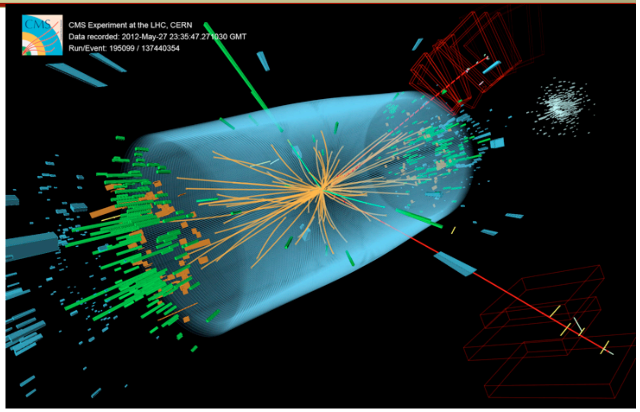
→**Better organization, faster access to news**

Scientific Discovery needs Fast Data Analysis

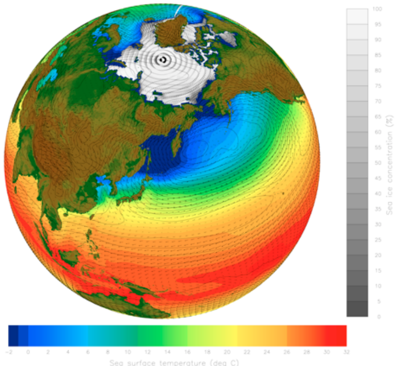
- **Modern scientific discoveries are driven by massive data**
  - Scientific simulations and experiments in many domains produce data in the range of terabytes and petabytes
- **Fast data analysis is an important requirement for discovery**
  - Data is typically stored as files on disks that are managed by file systems
  - High data read performance from storage is critical



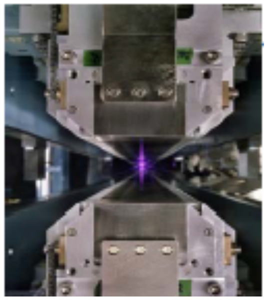
LSST image simulator



LHC: Higgs Boson search



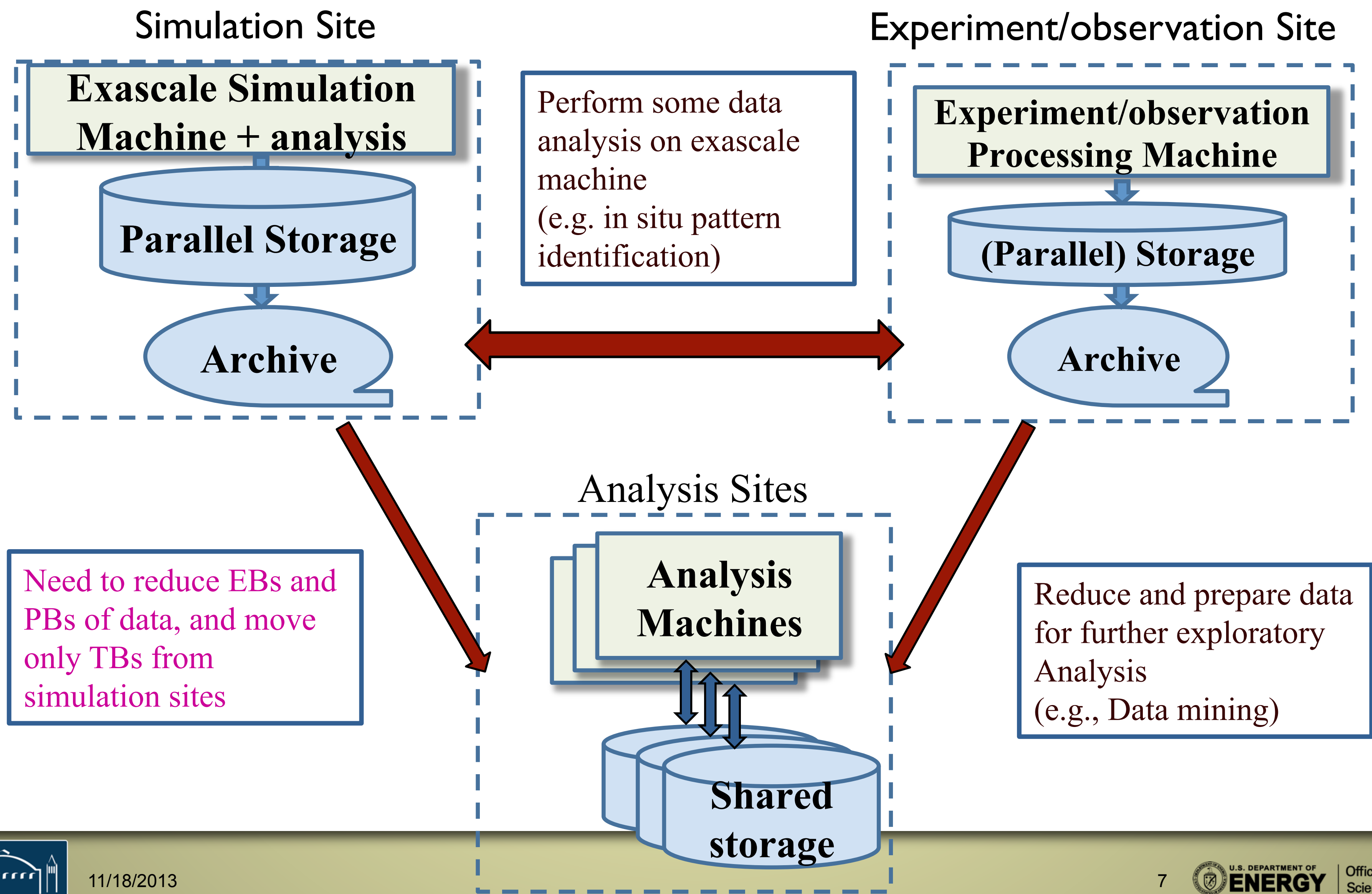
NCAR's CESM data



Light source experiments at LCLS, ALS, SNS, etc.

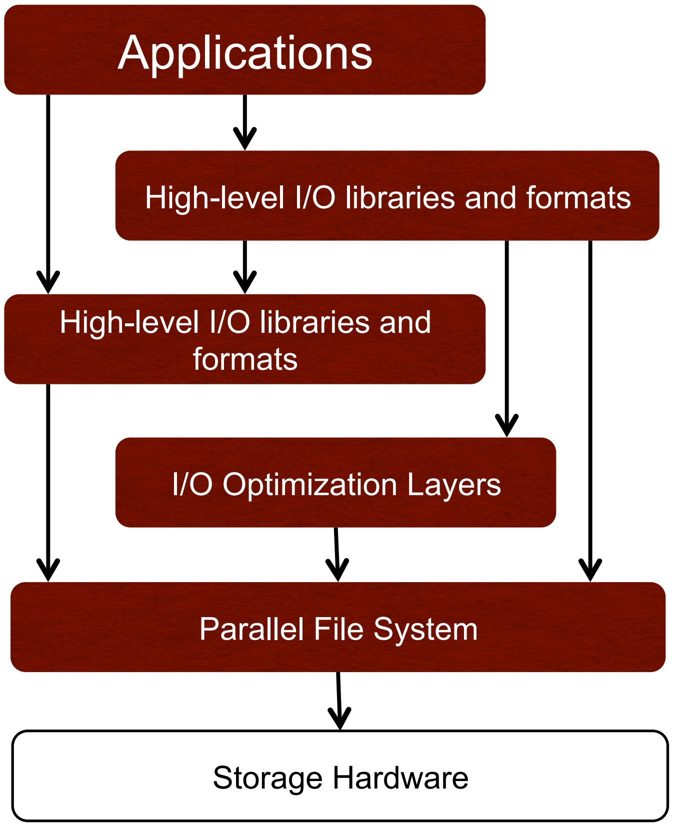
Image Credits
http://www.science.tamu.edu/articles/911
http://www.lsst.org/lsst/gallery/data
http://nsidc.org/icelights/category/research-2/

A Generic Data Analysis Use Case



Current Practice: Immutable Data in File Systems

- **Data stored on file systems is immutable**
  - After data producers (simulations and experiments) store data, the file format/ organization is unchanged over time
  - Data stored in files, which is treated by the system as a sequence of bytes
  - User code (and libraries) has to impose meaning of the file layout and conduct analyses
  - Burden of optimizing read performance falls on application developer
  - However, optimizations are complex due to several layers of parallel I/O stack



Parallel I/O Software Stack

Changing layout of data on file systems is helpful

- **Separation of logical and physical data organization through reorganization**
- **Example**
  - Access all variables where 1.15 < Energy < 1.4
  - Full scan of data or random accesses to non-contiguous data locations results in poor performance
  - Sorting the data and accessing contiguous chunks of data leads to good performance
- Several studies showing reorganization can help
  - Listed some in the related work section

Energy	X	Y	Z	…
1.1692	165.834	-28.0448	-2.76863	…
2.5364	166.249	-27.9321	-2.87165	…
1.4364	166.538	-27.9735	-3.16969	…
1.0862	166.663	-27.9769	-2.79716	…
1.2862	166.621	-27.9046	-2.78382	…
1.5862	167.001	-27.9366	-3.09605	…
1.3173	167.222	-27.9551	-3.22406	…

Changing layout of data on file systems is helpful

- **Separation of logical and physical data organization through reorganization**
- **Example**
  - Access all variables where 1.15 < Energy < 1.4
  - Full scan of data or random accesses to non-contiguous data locations results in poor performance
  - Sorting the data and accessing contiguous chunks of data leads to good performance
- Several studies showing reorganization can help
  - Listed some in the related work section

Energy	X	Y	Z	…
1.1692	**165.834**	**-28.0448**	**-2.76863**	…
2.5364	166.249	-27.9321	-2.87165	…
1.4364	166.538	-27.9735	-3.16969	…
1.0862	166.663	-27.9769	-2.79716	…
1.2862	**166.621**	**-27.9046**	**-2.78382**	…
1.5862	167.001	-27.9366	-3.09605	…
1.3173	**167.222**	**-27.9551**	**-3.22406**	…

Changing layout of data on file systems is helpful

- **Separation of logical and physical data organization through reorganization**
- **Example**
  - Access all variables where 1.15 < Energy < 1.4
  - Full scan of data or random accesses to non-contiguous data locations results in poor performance
  - Sorting the data and accessing contiguous chunks of data leads to good performance
- Several studies showing reorganization can help
  - Listed some in the related work section

Energy	X	Y	Z	…
1.0862	166.663	-27.9769	-2.79716	…
1.1692	**165.834**	**-28.0448**	**-2.76863**	…
1.2862	**166.621**	**-27.9046**	**-2.78382**	…
1.3173	**167.222**	**-27.9551**	**-3.22406**	…
1.5862	167.001	-27.9366	-3.09605	…
1.4364	166.538	-27.9735	-3.16969	…
2.5364	166.249	-27.9321	-2.87165	…

Database Systems for Scientific Data Management

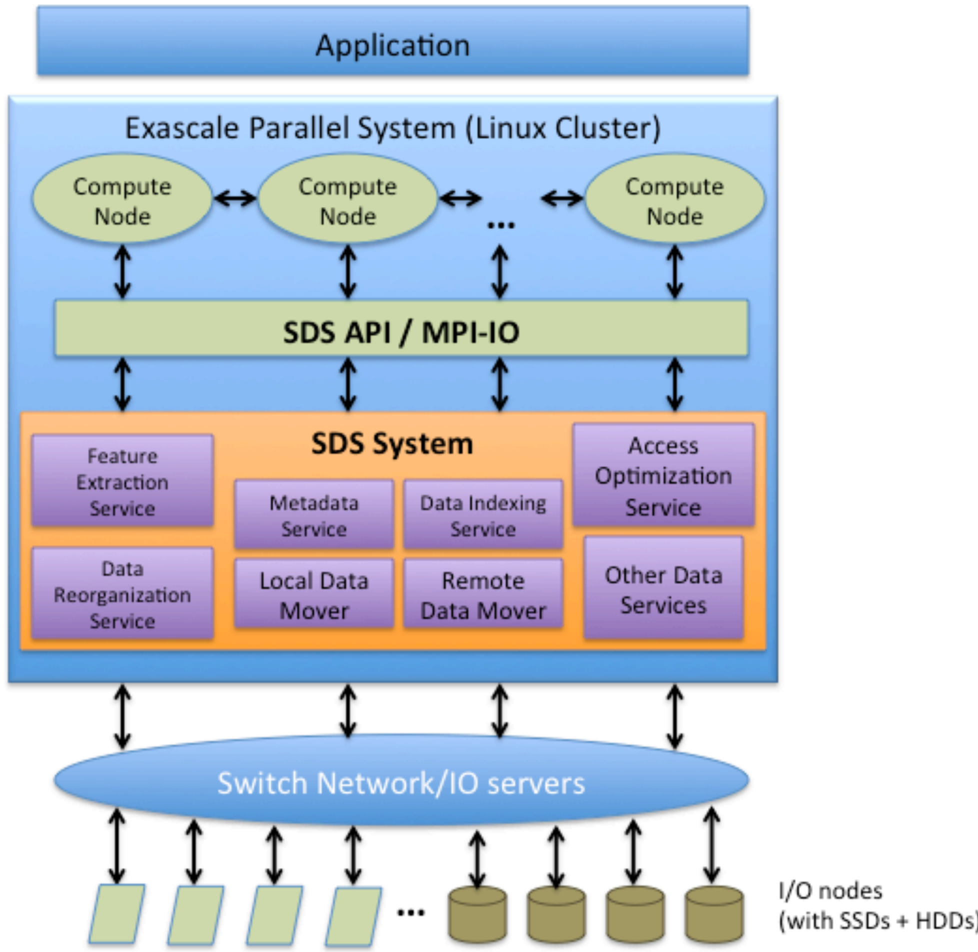
- **Database management systems perform various optimizations without user involvement**
- **Many efforts from database community reach out to manage scientific data**
  - Objectivity/DB, Array QL, SciQL, SciDB, etc.
- **SciDB**
  - A database system for scientific applications
  - Key features:
    - Array-oriented data model
    - Append-only storage
    - First-class support for user-defined functions
    - Massively parallel computations

More DB Optimizations, but …

- **Database systems use various optimization tricks and perform them automatically**
  - **Cache frequently accessed data**
  - **Use indexes**
  - **Store materialized views**
  - **…**
- **However, preparing and loading of scientific data to fit into database schemas is cumbersome**
- **Scientific data management requirements are different from DBMS**
  - Established data formats (HDF5, NetCDF, ROOT, FITS, ADIOS-BP, etc.)
  - Arrays are first class citizens
  - Highly concurrent applications

Our Solution: Scientific Data Services (SDS)

- **Preserving scientific data formats and adding database optimizations as services**
- **A framework for bringing the merits of database technologies to scientific data**
- **Examples of services**
  - Indexing
  - Sorting
  - Reorganization to improve data locality
  - Compression
  - Remote and selective data movement
  - …

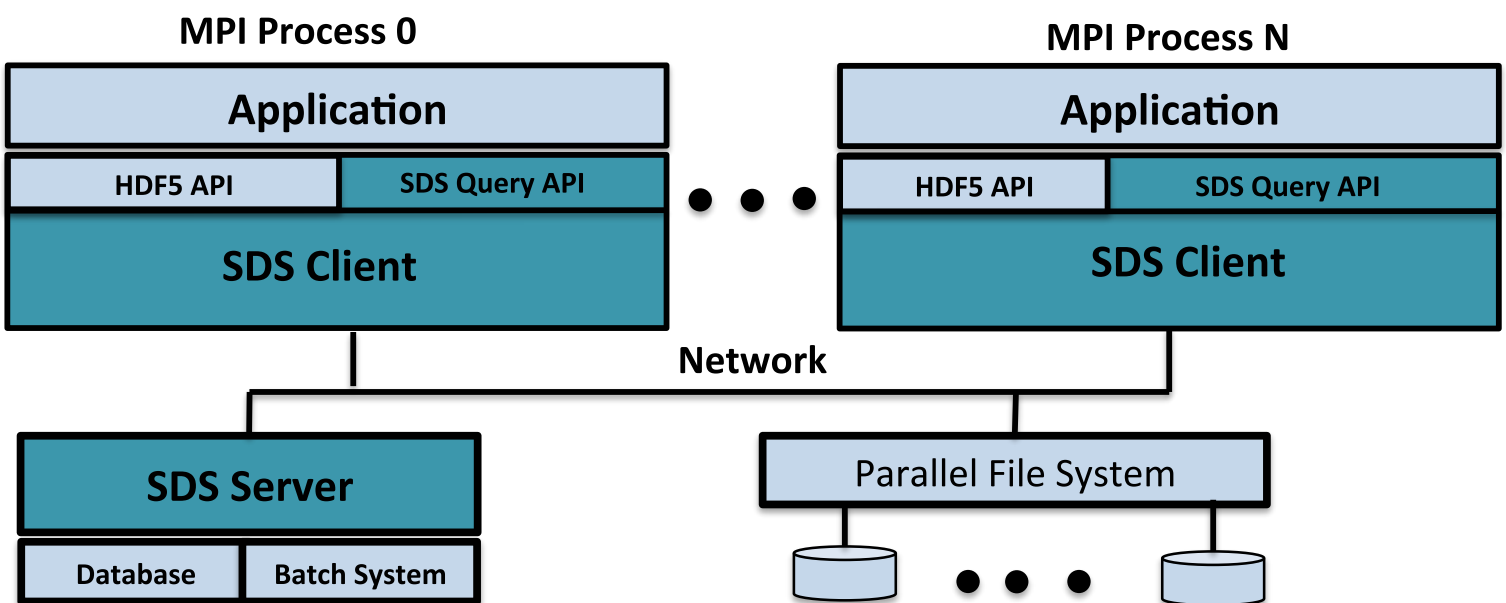


First step: Automatic Data Reorganization

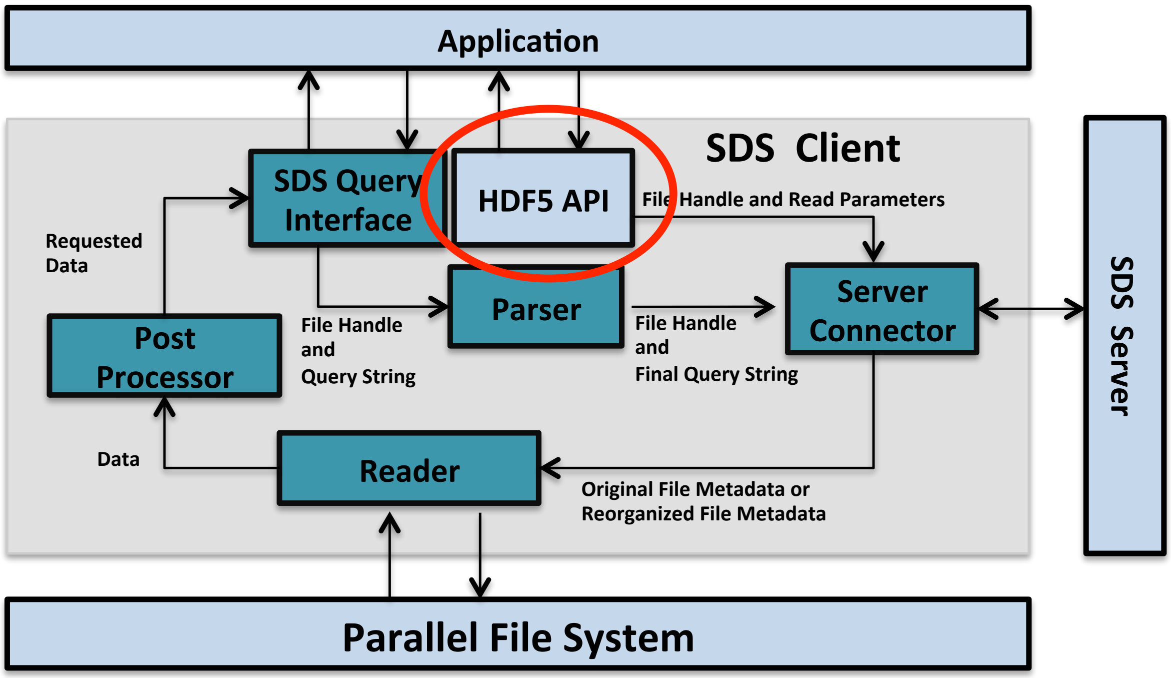
- **Finding an optimal data organization strategy**
  - Capture common read patterns
  - Estimate cost with various data organization strategies
  - Rank data organizations for each pattern and select the best for a pattern
- **Performing data reorganization**
  - Similar to database management systems, perform data reorganization transparently
  - Resolving permissions to the original data
  - Preserve the original permissions when data is reorganized
- **Using an optimally reorganized dataset transparently**
  - Based on a read pattern, recognize the best available organization of data
  - Redirect to read the selected organization
  - Perform any needed post processing, such as decompression, transposition

The Design of the SDS Framework

- **Initial implementation of the SDS framework**
  - Client-server approach
  - SDS Client library for each MPI process
  - SDS Server to find the best dataset from available reorganized datasets
  - Supporting HDF5 Read API
  - Added SDS Query API for answering range queries



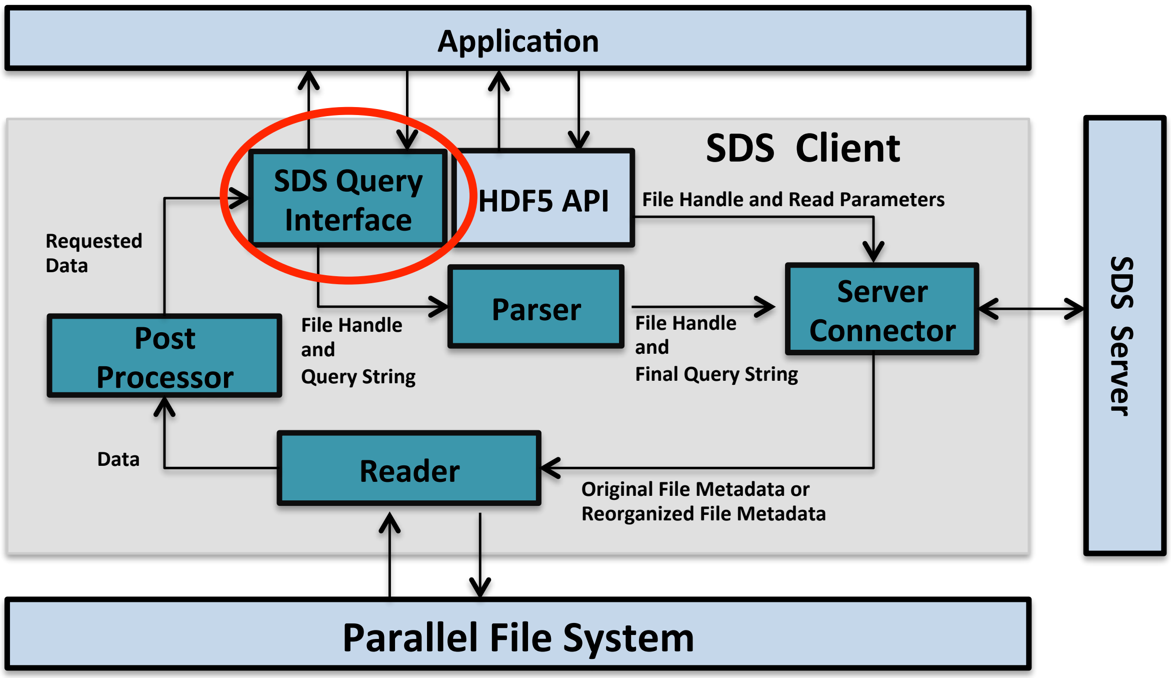
SDS Client Implementation



HDF5 API

- The HDF5 Virtual Object Layer (VOL) feature allows capturing HDF5 calls
- Developed a VOL plugin for SDS for capturing file open, read, and close functions

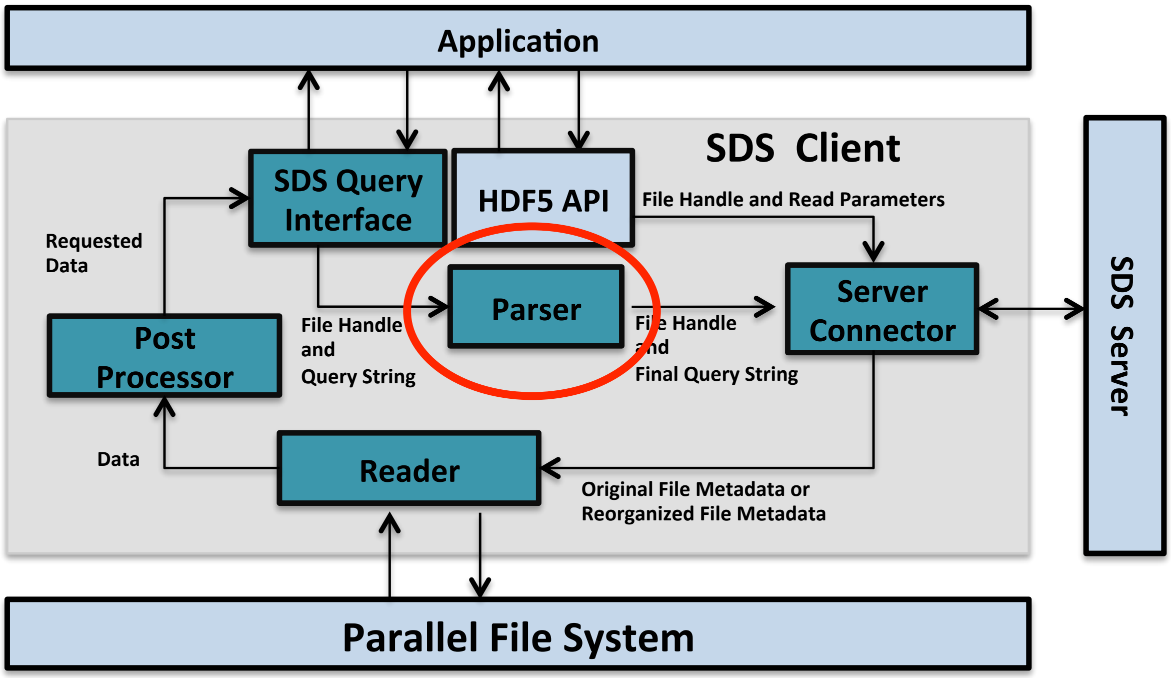
SDS Client Implementation



SDS Query Interface

- An interface to perform SQL-style queries on arrays
- Function-based API that can be used from C/C++ applications

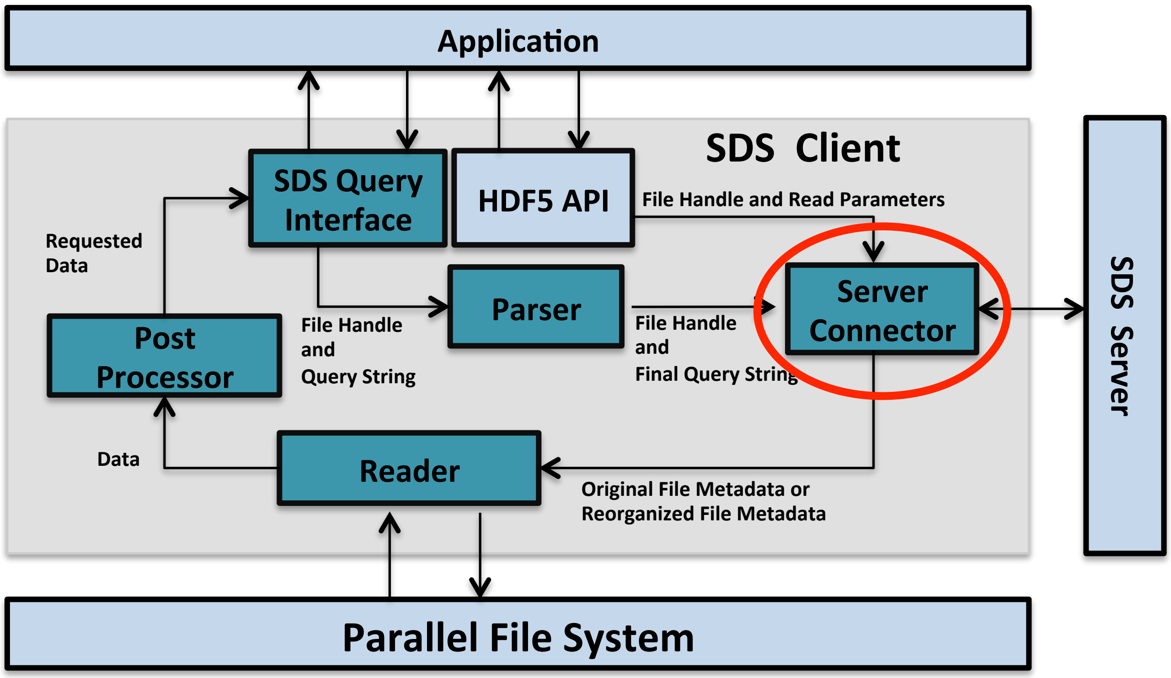
SDS Client Implementation



Parser

- Checks the conditions in a query
- Verifies the validity of files

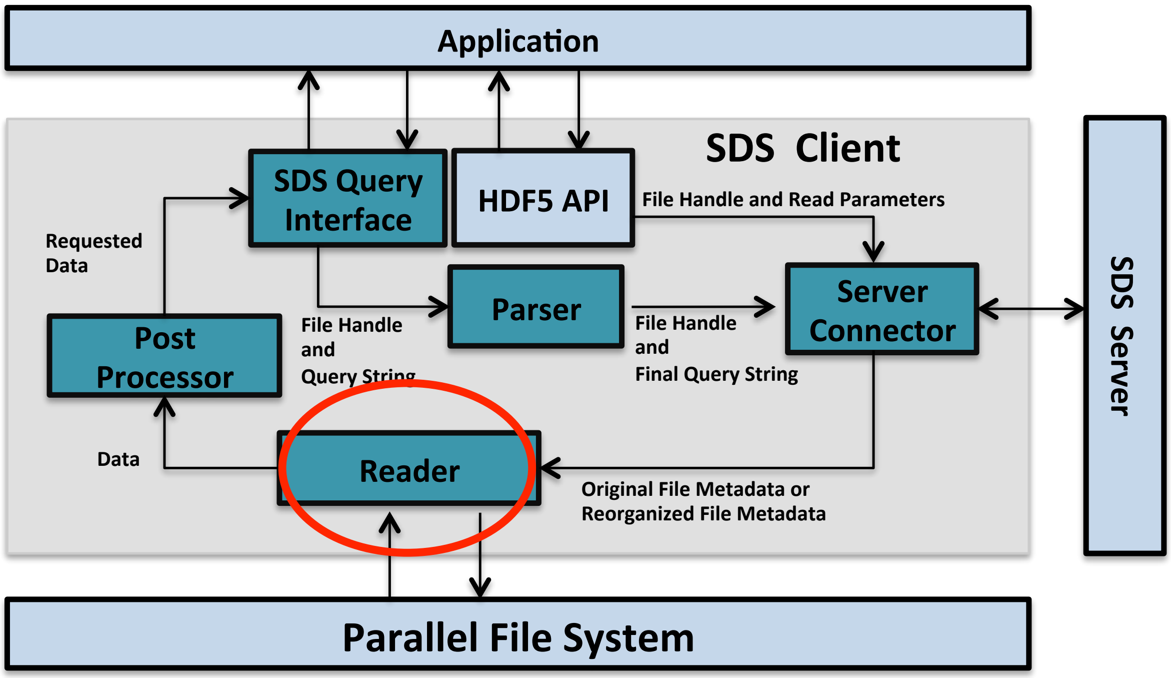
SDS Client Implementation



Server Connector

- Packages a query or HDF5 read call information and sends to the SDS server
- Using protocol buffers for communication
- MPI Rank 0 communicates with the server and then informs the remaining MPI processes

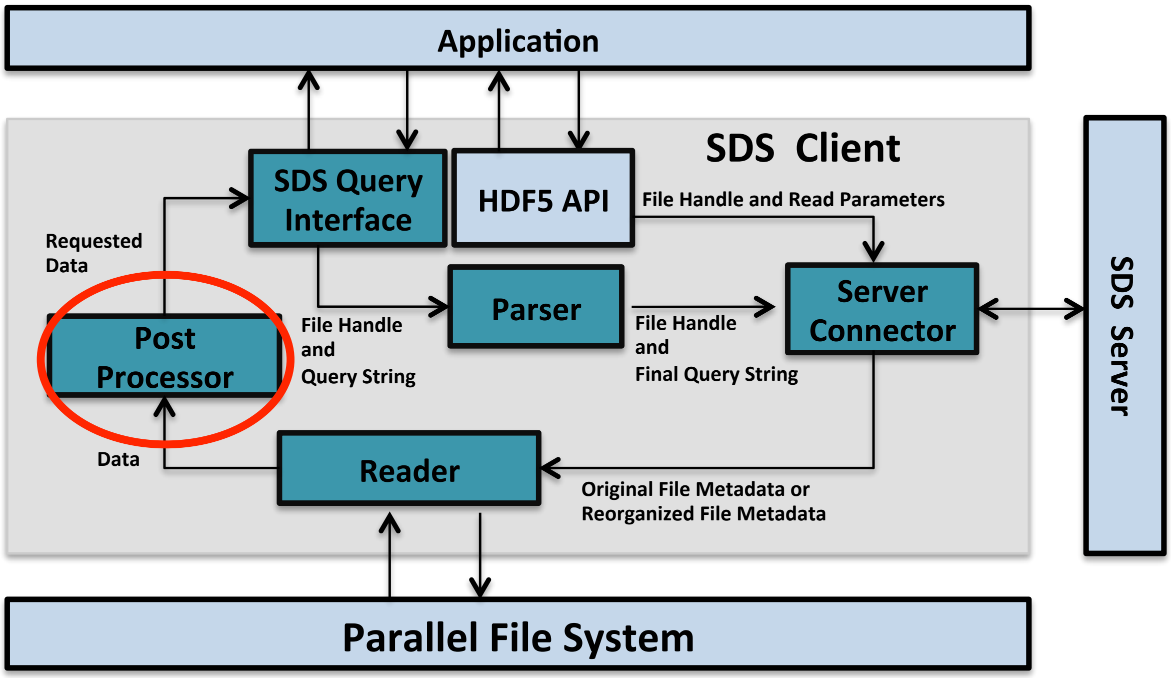
SDS Client Implementation



Reader

- Reads data from the dataset location returned by the SDS Server
- Makes use of the native HDF5 read calls

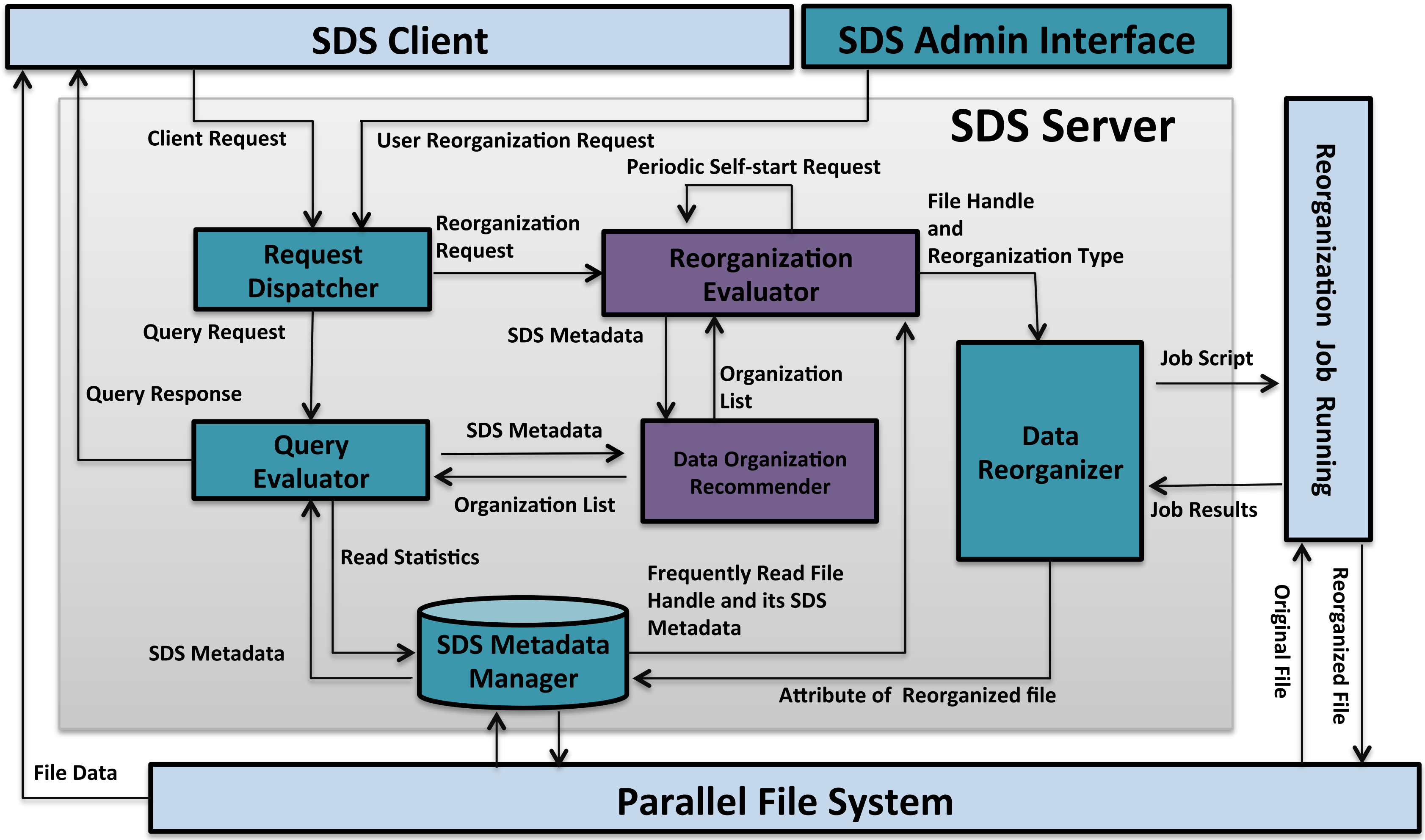
SDS Client Implementation



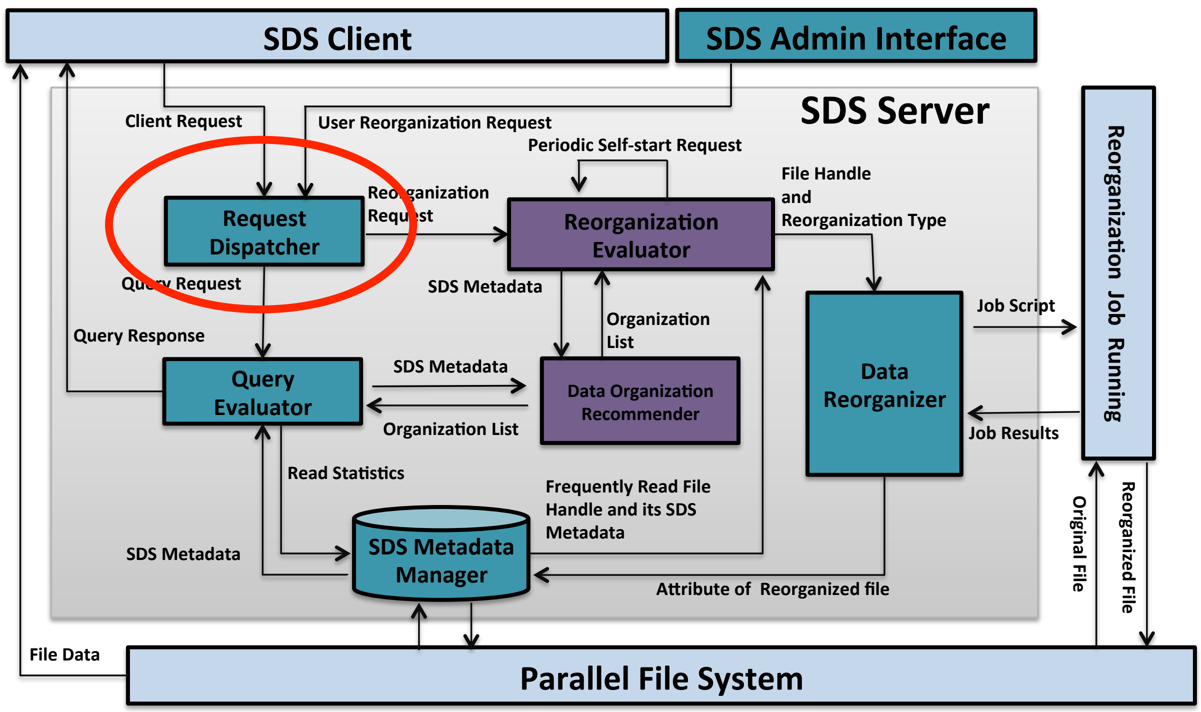
Post Processor

- Performs any post-processing needed before returning the data to the application memory
- Eg. Decompression, transposition, etc.

SDS Server Implementation



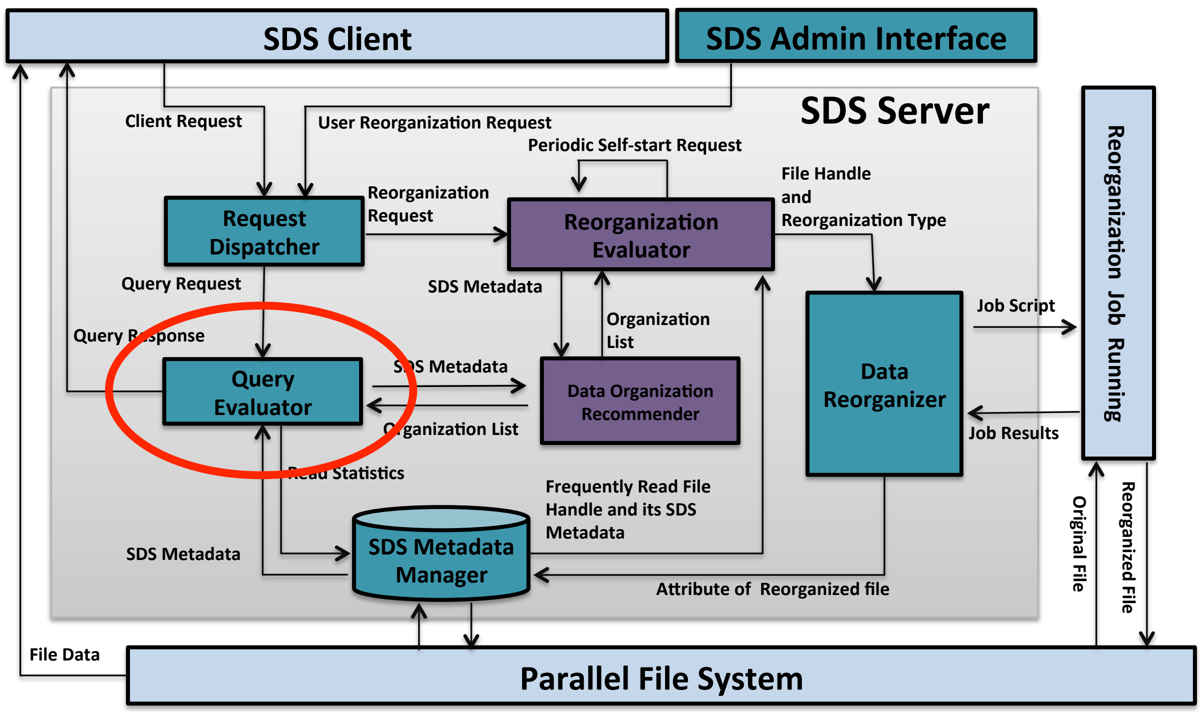
SDS Server Implementation



Request Dispatcher

- Receives SDS client requests and SDS Admin interface
- SDS Admin interface issues reorganization commands
- Based on the request, dispatcher passes on the request to Query Evaluator and Reorganization Evaluator

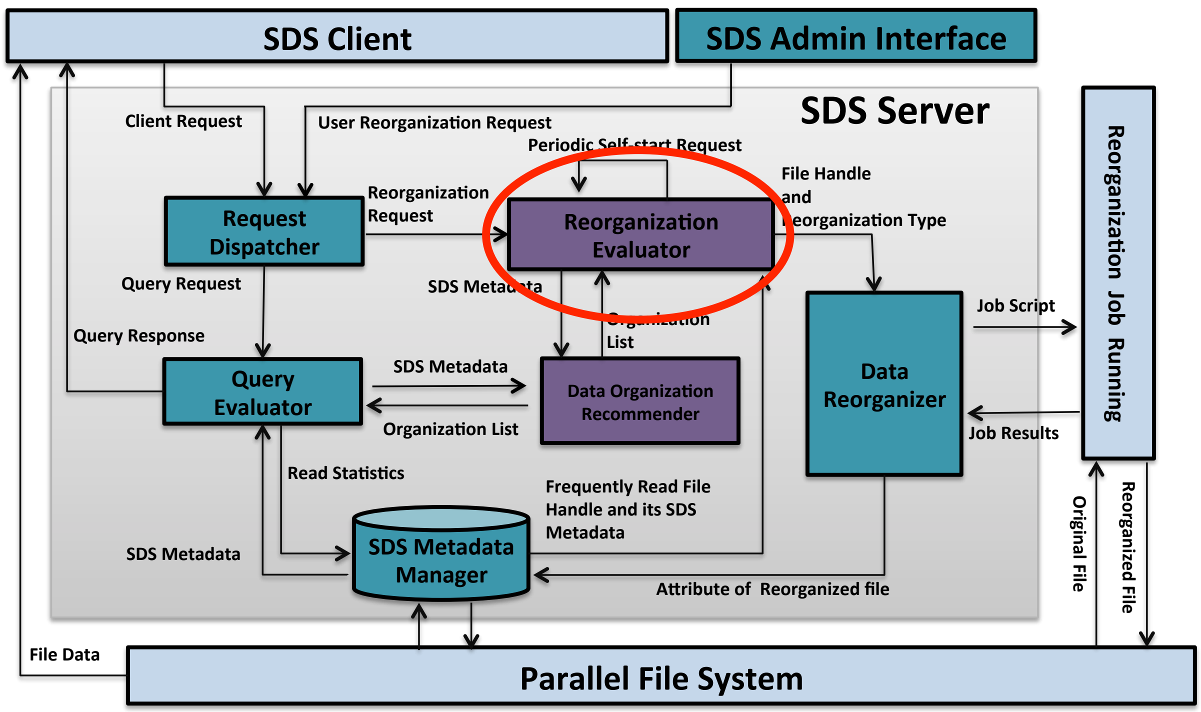
SDS Server Implementation



Query Evaluator

- Looks up SDS Metadata for finding available reorganized datasets and their locations for a given dataset
- SDS Metadata
  - File name, HDF5 dataset info, permissions

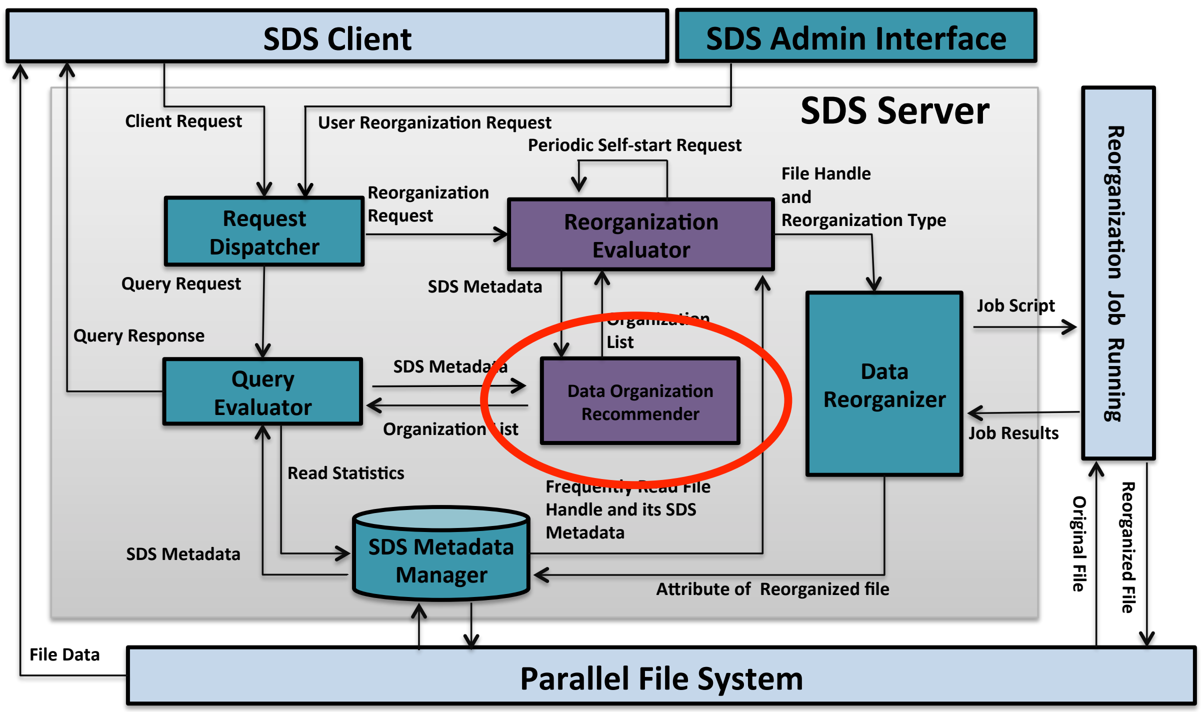
SDS Server Implementation



Reorganization Evaluator

- Decides whether to reorganize based on the frequency of read accesses
- Takes commands from the Admin interface
- Instructs Data Reorganizer to create a reorganization job script

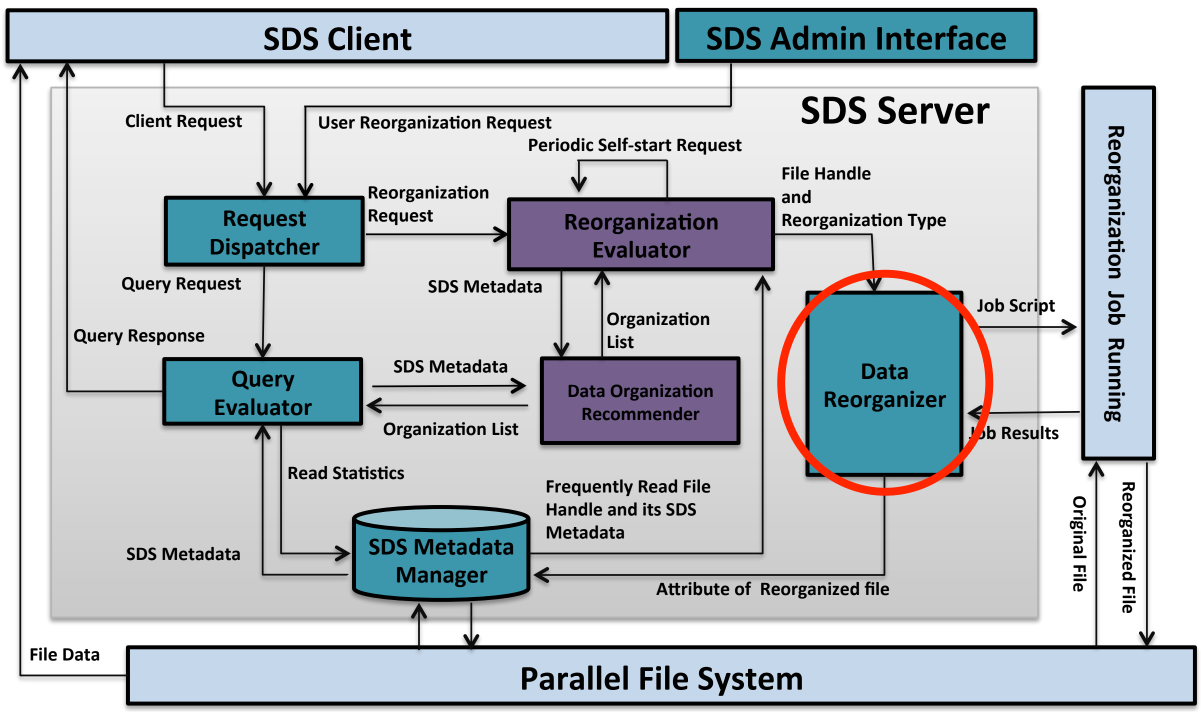
SDS Server Implementation



Data Organization Recommender

- Identifies optimal data reorganization
- Informs the Reorganization Evaluator with the selected strategy

SDS Server Implementation



Data Reorganizer

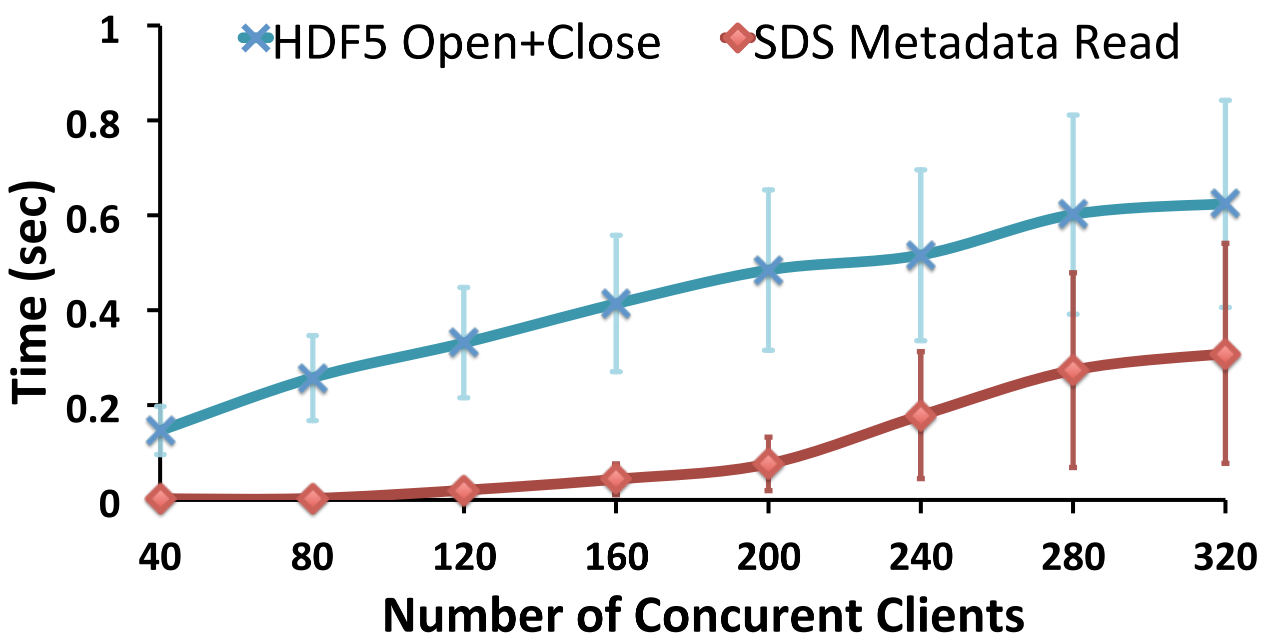
- Locates reorganization code, such as sorting, indexing algorithms
- Decides on the number of cores to use
- Prepares a batch job script
- Monitors the job execution
- After reorganization, stores the new data location in the SDS Metadata Manager

Performance Evaluation: Setup

- **NERSC Hopper supercomputer**
  - 6,384 compute nodes
  - 2 twelve-core AMD 'MagnyCours' 2.1-GHz processors per node
  - 32 GB DDR3 1333-MHz memory per node
  - Employs the Gemini interconnect with a 3D torus topology
  - Lustre parallel file system with 156 OSTs at a peak BW of 35 GB/s
- **Software**
  - Cray's MPI library
  - HDF5 Virtual Object Layer code base
- **Data**
  - Particle data from a plasma physics simulation (VPIC), simulating magnetic reconnection phenomenon in space weather

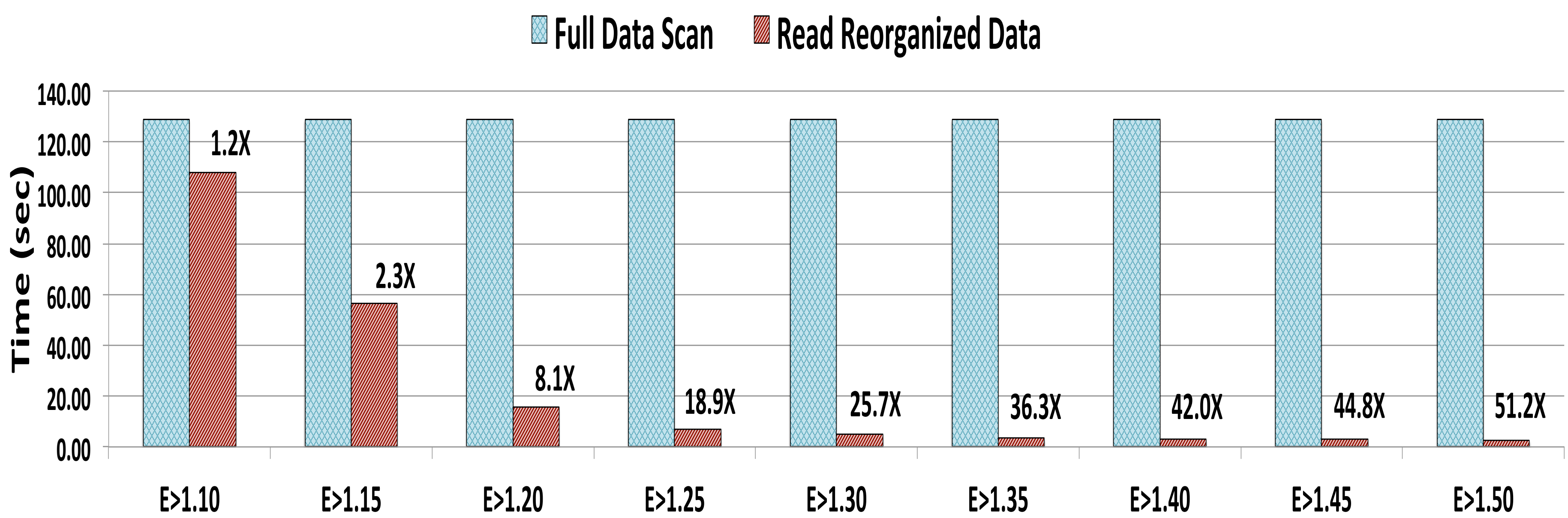
Performance Evaluation: Overhead of SDS

- SDS Metadata Manager uses Berkeley DB for storing metadata of reorganized data
- Measured response time of multiple concurrent SDS Clients requesting metadata from one SDS Server
- Low overhead of < 0.5 seconds with 240 concurrent clients



Performance Evaluation: Benefits of SDS

- Ran various queries on particle energy conditions
- Performance benefit over full scan varies based on selectivity of data
- 20X to 50X speedup when data selectivity less than 5%



Selectivity: 79% 32% 11% 4.6% 2.2% 1.2% 0.75% 0.5% 0.33%

Conclusion and Future Work

- **File systems on current supercomputers are analogous to print newspapers**
- **The SDS framework is vehicle for applying various optimizations**
  - Live customization of data organization based on data usage (in progress)
  - To work with existing scientific data formats
- **Status: Platform for performing various optimizations is ready**
- **Low overhead and high performance benefits**
- **Ongoing and future work:**
  - Dynamic recognition of read patterns
  - Model-driven data organization optimizations
  - In-memory query execution and query plan optimization
  - FastBit indexing to support querying
  - Support for more data formats

Thanks!

Contact: Suren Byna [SByna@lbl.gov]

Thanks to:

U.S. DEPARTMENT OF ENERGY | Office of Science

The HDF Group

NERSC