

SDS: A Framework for Scientific Data Services

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ABSTRACT

Large-scale scientific applications typically write their data to parallel file systems with organizations designed to achieve fast write speeds. Analysis tasks frequently read the data in a pattern that is different from the write pattern, and therefore experience poor I/O performance. In this paper, we introduce a prototype framework for bridging the performance gap between write and read stages of data access from parallel file systems. We call this framework Scientific Data Services, or SDS for short. This initial implementation of SDS focuses on reorganizing previously written files into data layouts that benefit read patterns, and transparently directs read calls to the reorganized data. SDS follows a client-server architecture. The SDS Server manages partial or full replicas of reorganized datasets and serves SDS Clients' requests for data. The current version of the SDS client library supports HDF5 programming interface for reading data. The client library intercepts HDF5 calls using the HDF5 Virtual Object Layer (VOL) and transparently redirects them to the reorganized data. The SDS client library also provides a querying interface for reading part of the data based on user-specified selective criteria. We describe the design and implementation of the SDS client-server architecture, and evaluate the response time of the SDS Server and the performance benefits of SDS.

General Terms

Scientific Data Services, I/O performance optimization, data reorganization, data layout optimization

Keywords

SDS, Scientific Data Services, SDS Framework

1. INTRODUCTION

Large scientific simulations and experiments typically store data to parallel file systems with a layout that gives the best performance for writing. Research efforts are underway to write data to parallel file systems, such as Lustre and GPFS, with the goal of achieving peak I/O bandwidth [3, 1]. The stored data is frequently distributed

to many users around the world for further analysis. It is common for some of the analysis tasks to read data in a different pattern that does not match the write pattern. For example, simulation data is typically written out one time step at a time, while many analyses read data records from a spatial region over time. Such read operations are much slower than contiguous read operations.

Difference in read and write access patterns also exists in other applications such as database systems. Relational database management systems improve the read performance through techniques such as using indexes, caching frequently accessed data, and storing materialized views. These optimizations are invisible to database users. However, with scientific data, once the data is stored to a file system, the data becomes immutable, and users have to implement read optimizations in their own application code. The aim of this work is to bring the automatic data management features from database community to scientific data stored in files [14].

Reorganizing data is a proven strategy for improving read performance. Methods such as elastic data reorganization (EDO) [11], 2-D layout [10], and multi-dimensional chunking [9], have been shown to work well for specific data access patterns. Our recent study also shows that accessing sorted or transposed data layout speeds up reading data by more than 50X [6].

Different access patterns generally require different data organizations, creating the appropriate organization requires extensive knowledge about the complex parallel I/O subsystems. Furthermore, managing the reorganized copies requires extensive knowledge about the file system. Encapsulating these operations into an automated system for the reorganized data could significantly improve the performance of data analysis tasks and accelerate scientific discovery.

Ultimately, we plan to develop a scientific data management system that achieves the peak I/O bandwidth for both write and read operations. In this paper, we describe our first step towards that overarching goal: the design and an initial implementation of the Scientific Data Services (SDS) framework. We first analyze the requirements involved in the automatic data reorganization process and identify the key requirements for implementing a data reorganization system. We then present our initial implementation of SDS, which is a new lightweight client-server based framework for reorganizing files stored on parallel file systems. Specifically, SDS is able to automatically identify the files that need to be reorganized and to invoke an appropriate data reorganization algorithm (such as sorting and/or transposing the data), and to reorganize the files accordingly. SDS currently supports HDF5, a popular high-level I/O interface, for reading the optimally reorganized data files. To perform transparent redirection of HDF5 read calls, we have implemented a new HDF5 Virtual Object Layer (VOL) plug-in that intercepts the HDF5 calls and directs them to SDS organized files.

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We have also introduced a new interface, called SDS Query, for querying the data that satisfies given range conditions. The following are the contributions of this work.

- We discussed the requirements of developing an automatic data reorganization framework.
- We introduced the design and the implementation details of the SDS framework.
- We evaluate the overhead of using the SDS framework and the performance benefits with SDS.

This rest of the paper is organized as follows: we review the requirements for the automatic reorganization of data in Section 2. In Section 3, we describe the design and implementation details of the SDS framework. Section 4 discusses the experimental set up for evaluating the SDS framework and Section 5 presents the measurements of overhead of using SDS and the resulting read performance. Section 6 reviews related work and Section 7 concludes the paper with a brief discussion of future work.

2. REQUIREMENTS OF AUTOMATIC REORGANIZATION

2.1 Finding optimal organization

Determining an optimal organization of data for accelerating read operations has been explored by several research activities [10]. A typical strategy is to identify data read patterns of analysis applications, and then to determine an organization that improves the locality and parallelism of the data access from the file system. The reorganized data may include one or more copies of the original data. To minimize the storage space requirement, it is important to replicate only the most useful information. For example, if the analysis operations only need a part of a data set, then we should avoid replicating the whole data set. In this paper, we assume the read patterns and their corresponding optimal organizations are known. We focus on providing a mechanism for performing a selected reorganization and for directing read calls to the reorganized datasets.

2.2 Performing reorganization

Given a specific organization, to produce a reorganized copy requires us to consider a few practical issues. First, an automatic reorganization system needs the permission to read the original data and to protect the reorganized data. Scientific data is often produced by a user or a group of users and sharing of that data is limited by the owners. A reorganization system needs to respect the established permissions. Second, the system has to read the data and perform the reorganization, such as sorting and transposition, and to write the data to the file system efficiently. This step requires computing power and memory resources. To perform this automatically on machines that run jobs in a batch mode, a reorganization system needs to submit batch jobs automatically. Third, after a reorganization job is finished, the system needs to manage the reorganized data and its associated metadata for future read requests. The replicated data also needs to be protected by giving permissions only to the owners of the data. We will describe the implementation for performing data reorganization with our SDS framework in Section 3 addressing these issues.

2.3 Reading reorganized data transparently

Assuming there are multiple replicas of data in different layouts on a file system, we need to redirect each read request to a replica

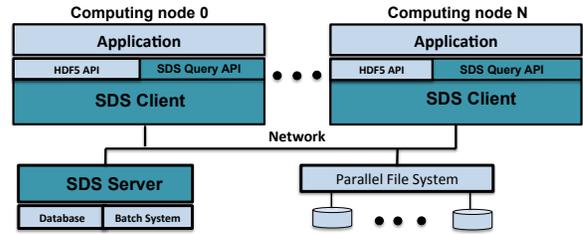


Figure 1: An Overview of SDS Framework

that gives the best read performance. This task has three challenges: selecting a replica of data to achieve the best performance for a read pattern, intercepting a read call, and redirecting the call to the selected data. Finding the best performing data organization is similar to the requirement mentioned above in Section 2.1.

A reorganization system needs to recognize the pattern of one or a set of read calls at runtime and match the logical pattern with physical layout that will provide the best performance. This is a challenge we will be addressing in our future work. This paper focuses on solving the second and third challenges: intercepting read calls and directing them to read the data layout that will provide the best performance.

3. SCIENTIFIC DATA SERVICES

In this section, we provide an overview of the Scientific Data Service (SDS) framework. The current implementation includes functions to perform specified reorganizations and redirecting read operations to appropriate copies of the data.

3.1 SDS Framework Overview

Figure 1 shows a high-level overview of the SDS framework. SDS has two main components: the SDS Server and the SDS Client.

The SDS Server performs reorganization of the data, manages the metadata of the reorganized datasets, and handles the requests from SDS Clients to identify the best version of reorganized dataset to use. The Server handles multiple SDS Clients related to different applications, simultaneously.

The SDS Client is a light-weight library responsible for intercepting data read calls and for contacting the SDS Server for the location of data to be read. MPI (Message Passing Interface) application processes linked with the SDS Client library read the data directly from the parallel file system and perform any mapping needed between the reorganized data and the read request. Our current implementation supports reading of data through HDF5 library. HDF5 is a popular data format used by numerous scientific applications for reading and writing multi-dimensional array data. In addition to HDF5 read calls, the SDS Client also supports range queries through the SDS Query interface. With this interface, applications can request to access data with an SQL like query, such as “var1 > value1 and var2 <= value2”.

3.2 SDS Server Design and Implementation

Figure 2 shows an overview diagram of the SDS Server. The server contains the following components: Request Dispatcher, Query Evaluator, Reorganization Evaluator, Data Organization Recommender, Data Organizer, SDS Admin Interface, and SDS Metadata Manager. We now explain each of these components.

- The *Request Dispatcher* handles requests from SDS Clients and the SDS Admin Interface. The clients send metadata requests to verify whether there are any reorganized data files

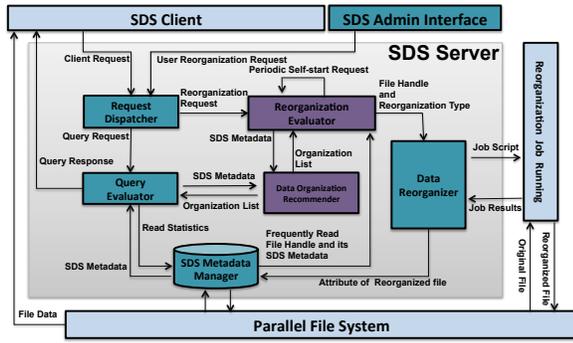


Figure 2: Design of the SDS Server and interactions among various components. Reorganization Evaluator and Data Organization Recommender are implemented partially and the other highlighted components are implemented fully.

related to a read request and to obtain metadata of the reorganized data files, such as the reorganized data file name, offsets, sizes of the data to be read, etc. We have developed an SDS Admin Interface for issuing data reorganization requests. Ideally, the SDS Server should be capable of making intelligent decisions on finding data organizations based on known read patterns. However, at this initial stage, we use the Admin interface for providing well-known data organization decisions to the Server. We implemented the communication between the client and the server using protocol buffers or protobuf [12], a message interchange format provided by Google. The client or the Admin Interface sends requests comprising of file name, dataset name, query or coordinates of the array variable, and the type of the request (read, query, or reorganization) encoded into a protobuf message. The Request Dispatcher decodes the message; based on the type of request it dispatches the request either to the Query Evaluator or to the Reorganization Evaluator.

- The *Query Evaluator* analyzes the metadata requests from SDS Clients and performs a lookup for existing reorganized datasets in the *SDS Metadata Manager*. The Metadata Manager maintains relationships between the original data files and their reorganized datasets. Typical SDS metadata includes the name, file location, group name, dataset name for both the original and the reorganized files, and the permissions of the datasets. To ensure the security of the reorganized file, the original file's access permissions for both user id and group id are stored in the SDS metadata. We also store the read statistics including the frequencies and access patterns for each file. We store the SDS Metadata Manager using Berkeley DB. The Query Evaluator uses a thread pool to provide concurrency while control the resource usage. The Query Evaluator is capable of supporting numerous SDS Clients simultaneously. Each thread handles one client request for looking up reorganized datasets, verifying permissions, and sending the location of reorganized file to the client. The Query Evaluator encodes the metadata using protobuf and sends that information to the client.
- The *Reorganization Evaluator* is responsible for deciding whether to reorganize data based on the frequency of access to a dataset and for handling reorganization requests that come from the SDS Admin Interface. It periodically checks the SDS metadata for the most frequently accessed

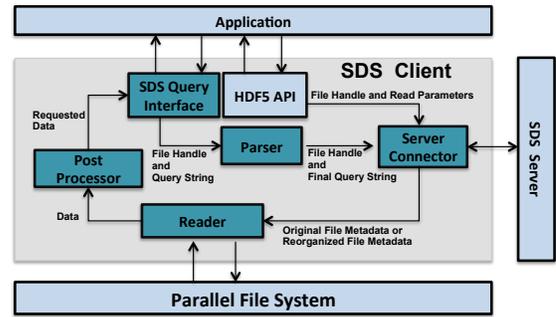


Figure 3: An overview of the SDS Client and the interactions among various components

data files and their read patterns for deciding the need for reorganization. The Reorganization Evaluator also utilizes the *Data Organization Recommender* in selecting the best organization when multiple reorganized files are available. The current implementation supports the requests from the SDS Admin Interface.

- Based on known read patterns and the original layout of the data on the file system, the *Data Organization Recommender* selects the optimal layout and suggests the Reorganization Evaluator to perform the reorganization. This component evaluates the logical view of the read requests and physical data layout of the data for satisfying the read requests, and estimates the latency with various possible physical layouts. We are currently developing a model for choosing optimal data layout.
- The *Data Reorganizer* performs the selected reorganization task. It initiates a reorganization method by generating a batch script to run on a large computer system. We currently support two types of reorganization methods: parallel sorting and transposition. We have shown the benefits of these two data organization methods for two scientific datasets [6]. The SDS Admin Interface is designed to support other reorganization functions to be added in the future. The Data Reorganizer also monitors the health of a reorganization script and after executing the script, it stores the reorganization related metadata into the SDS Metadata Manager database.

3.3 SDS Client design and implementation

Figure 3 shows an overview of the SDS Client architecture. The client library supports two types of read interfaces: the HDF5 Read API and SDS Query Interface. The Parser parses the data query request conditions of the Query Interface and the Server Connector communicates with the SDS Server. We implemented the current SDS Client library using the Virtual Object Layer (VOL) of the HDF5 library [4]. The VOL supports a mechanism for intercepting HDF5 calls. Our recent paper [6] provides details of our VOL plugin implementation.

- *SDS Query Interface*. The SDS Query Interface provides users the ability to run SQL-style queries on arrays. We extend the HDF5 Read API to accommodate the querying conditions on the specified dataset. The Query API supports returning the count of the data elements satisfying a condition and returning the results of the query to the application.
- The *Parser* verifies query requests for validity, such as whether the requested data file and dataset exists. The Parser passes

the attributes of the query conditions to the SDS Server for finding the location of a file organized by the requested dataset. In our current implementation, the execution of the SDS Query depends on whether a dataset being queried is sorted or not. Answering queries with the help of indexes is under development.

- The *Server Connector* packages either a query or a HDF5 read request into a protobuf data structure and sends it to the SDS Server for retrieving information including the location of the data to be read. In a parallel application using MPI, the SDS Client with MPI Rank 0 sends the request to the SDS server. This strategy avoids all processes of the application asking for the same information from the SDS Server. After the Server Connector on Rank 0 has received the metadata information from the server, it broadcasts the information to all other MPI processes of the application.
- The *Reader* issues HDF5 Read calls based on the metadata information on the location of the dataset. We implemented this as part of the HDF5 VOL with native HDF5 plugin, where HDF5 data is read from the parallel file system.
- When reorganizations such as compression or transposition to a different dimension are performed to achieve better performance, the reorganized data needs to be decompressed or transposed back when the data is returned to the application [6]. Based on the reorganization type, the *Post Processor* performs transformations to present the data in a way that the application expects.

4. SYSTEM CONFIGURATION

We have tested our initial implementation of the SDS framework on a Cray XE6 supercomputer at the National Energy Research Scientific Computing Center (NERSC), named Hopper¹. The system has 6,384 compute nodes, with two 12-core AMD ‘MagnyCours’ 2.1 GHz processors and at least 32 GB memory per node. We used a Lustre file system, exported as directory `/scratch2`, for storing and reading data.

To have a static IP address and port number to serve the SDS Client requests, we ran the SDS Server daemon on a Node Manager (MOM)² of the Hopper system. The SDS Server submitted reorganization job scripts to run on Hopper. Using the SDS Admin Interface, we manually initiate the reorganization requests.

5. RESULTS

In this section, we evaluate the response time of the SDS Server in handling concurrent SDS Client requests and the performance benefit in reading data using the SDS Client library.

5.1 SDS Metadata Read Response Time

In our current deployment on Hopper, we used one SDS Server. We measured the server response time with the number of SDS Clients varying between 40 and 320. We also measured the time for opening and closing HDF5 files with the same number of clients. In both cases, each SDS Client accesses a different file. The SDS Server reads the requested metadata related to a dataset from a database managed by Berkeley DB and returns it to SDS Clients.

¹<http://www.nersc.gov/systems/hopper-cray-xe6/>

²<https://www.nersc.gov/users/computational-systems/hopper/configuration/support-nodes/>

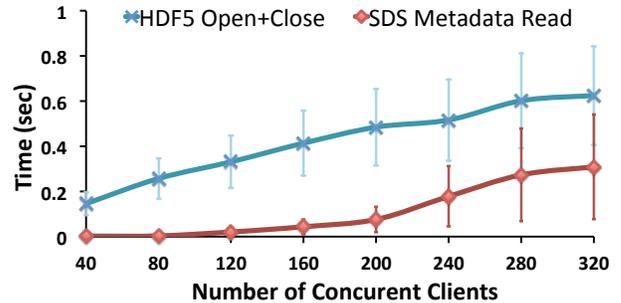


Figure 4: SDS Metadata Read Overhead from SDS Server

Figure 4 compares the response time of SDS with the time spent for HDF5 Open and Close operations by the same number of clients. The x-axis shows the number of clients and the y-axis shows the time in seconds. Each data point refers to the average response time with a range bar showing minimum and maximum response times. The maximum response time of SDS is less than 0.1 seconds in handling up to 200 clients and increases to ≈ 0.5 seconds in responding to 320 clients. In the same figure, we also show the time needed to perform HDF5 Open and Close operations. It is easy to see that the time needed for SDS to look up the metadata is considerably smaller than the time needed to open and close the HDF5 files. On Hopper, the average number of concurrent applications is ≈ 250 . In a production deployment, we expect the number of applications using SDS to be close to a few 10’s and therefore the overhead will be negligible.

5.2 Performance of Reading Reorganized Data

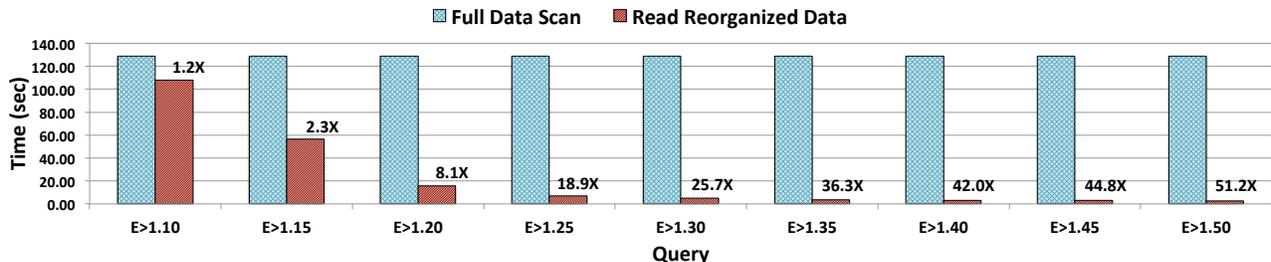
To show the effectiveness of using the SDS Client in reading a reorganized dataset, we performed range queries on a large plasma physics dataset. In [6], we have shown that sorting and querying this dataset gives up to 50X performance benefit compared to the traditional way of reading and sifting through the whole dataset for a given query condition. In this paper, we use the new SDS Client and Server implementation to verify that we are achieving similar performance benefits. In other words, the overhead introduced by the prototype implementation is minimal.

In these tests, we use a 2.8TB plasma particle dataset generated by our VPIC simulation [3]. The data contains seven variables: Energy, X, Y, Z, $U_{||}$, $U_{\perp,1}$, and $U_{\perp,2}$. The properties of all the particles is written into a HDF5 file based on X, Y, and Z location. We used the SDS Admin Interface for sorting this dataset based on Energy values using our parallel sorting algorithm explained in [6]. We ran multiple queries on this data with different ranges of Energy values to retrieve particles with a certain Energy threshold, which is a typical query for analyzing this data. The traditional approach of searching for energetic particles is a ‘Full Scan’, where an analysis application reads all the data variables into memory and then selects those where particle energy satisfies a given condition. With the SDS Query interface, we can specify the query condition and read the sorted file only where the energy value condition applies. Table 1 shows the query conditions, the size of data that satisfies the condition, and the percentage of data to be read from the total dataset. For a query of $E > 1.1$, $\approx 78\%$ of the data needs to be read and for $E > 1.5$, $\approx 0.3\%$ of the data is accessed.

Figure 5 shows the performance benefit of querying data with SDS, where the SDS Client requests the Server for the location of an optimal layout of the original data, and reads from a sorted dataset. The full scan of data takes the same time for all cases, as

Table 1: Size of the data extracted by each query from a 2.8TB VPIC data set

	$E > 1.10$	$E > 1.15$	$E > 1.20$	$E > 1.25$	$E > 1.30$	$E > 1.35$	$E > 1.40$	$E > 1.45$	$E > 1.50$
Size (GB)	2213.94	904.63	319.85	131.31	63.31	35.00	21.43	13.96	9.35
Percentage(%)	78.67	32.14	11.36	4.66	2.24	1.24	0.76	0.49	0.33

**Figure 5: Reorganized file performance benefit on a 2.8TB VPIC dataset**

the main cost is reading the data from disk and searching for the data that satisfies a given condition takes a negligible time. In comparison, SDS reads a fraction of the data that satisfies the condition. As the amount of data to be read becomes smaller, the performance benefit increases. We observed 20X to 50X speed up with SDS compared to the traditional full scan method when $\approx 5\%$ or less of the data satisfies the query condition.

6. RELATED WORK

Matching the file organization to the data access pattern can improve the data access performance. For a known access pattern, one could usually define a custom file organization. These efforts can be performed at system-level and at file-level. Typically, through sophisticated file allocation strategy, the system-level method minimizes variance of I/O servers [8], improve load balance [15, 16], and reduce I/O contention [7]. The granularity of file-level organization includes striping, disk blocks and so on. Typical file-level organizations include EDO [11], 1-DV[10], 1-DH [10], 2-D layout [10] and multidimensional chunks [9]. In most cases, these are static methods, where the file organization is determined when they are written to the file systems.

Recently, the ability to query scientific data similar to that of database management systems became an active research field. One idea is to load scientific data into special databases, and then apply a specially designed query language to find data of interest. An example of such an approach is SciDB [2], which provides query and functional languages for querying the data. In most cases, loading scientific data into SciDB is a laborious and time consuming effort. Furthermore, scientists wish to have access to their preferred file format, such as HDF5 or NetCDF. Another set of efforts is focused on building a querying system directly on the raw scientific data files. Typical examples include FastQuery [5, 3], an array-based querying library based on FastBit [13] and FlexQuery [17]. These efforts do not perform reorganization of data based on patterns.

7. CONCLUSIONS AND FUTURE WORK

Scientific data once written to parallel file systems with a certain data layout becomes immutable. The read performance of subsequent analysis tasks is poor when the read patterns differ from the write patterns. In this paper, we discuss the design and implementation of an automatic data optimization framework for reorganizing and augmenting the original data. We have shown the perfor-

mance overhead of our framework is minimal and the benefit is in the range of 2X to 50X.

We are exploring several aspects of improving the initial implementation of the framework. As mentioned in Section 2, determining an optimal organization of data automatically by matching the logical data access patterns with physical layout of the data is underway. Replication of the full dataset is a typical practice in Hadoop based systems. However, replicating petabytes of scientific data is impractical due to storage limitations. We are exploring methods to limit the replication to frequently accessed data. We are also expanding querying to complex conditions which can benefit for indexing. We plan to use bitmap indexes computed by FastBit technology [13].

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