

SIRIUS: A Revolutionary Approach to I/O and Storage for Exascale Scientific Computing

Jay Lofstead^{*}, Hasan Abbasi[‡], Mark Ainsworth^{||}, Jong Choi[‡], Matthew Curry^{*},
Scott Klasky^{§*}, Tahsin Kurc^{‡‡}, Qing Liu[‡], Jeremy Logan[§], Carlos Maltzahn[†], Manish Parashar[¶],
Norbert Podhorzski[‡], Feiyi Wang[‡], Matthew Wolf^{**}, C. S. Chang^{††}, Michael Churchill^{††}, Stephane Ethier^{††}
^{*}Sandia National Laboratories, [†]University of California Santa Cruz,
[‡]Oak Ridge National Laboratory, [§]U. Tenn. Knoxville, [¶]Rutgers University,
^{||}Brown University, ^{**}Georgia Tech, ^{††}PPPL, ^{‡‡}Stony Brook

Abstract

The longest existing parallel I/O APIs, HDF5, PnetCDF, and NetCDF, are focused on treating the entire output from a parallel application as a single unit. These libraries work to gather the data from all processes and arrange it such that it is organized much like as if it were written from a single process. This approach, in particular the two-phase collective I/O with data sieving portion, has proven difficult to scale for 3-D domain decompositions at scale. ADIOS shifted the focus from treating the entire application output as a single entity to treating the output from each writer as a self-contained entity. This eliminated the need for the problematic two-phase collective I/O and has demonstrated good scalability well into the petascale era. Another shift is required to address the needs of exascale systems. New supercomputing system I/O bandwidth is not keeping pace with the compute acceleration leading to accute bottlenecks. While “burst buffer” technology will help address the performance gap, it does not address the problem completely. This paper describes a new approach to not just an I/O library, but also the underlying storage infrastructure to address the needs of exascale applications cognizant of projected exascale platform characteristics and in the context of current industry trends.

1 Introduction

High performance computing simulations have driven tightly coupled platform scaling for decades. The output from these simulations are analyzed using regular tools and techniques optimized for this environment. The first generation of standardized APIs for scientific computing IO focused on serial output from a single process to a distributed or local file system. These systems still exist in the form of serial HDF5 [4] and the end-of-life NetCDF 3.x [14]. The key feature of these APIs is the logical data model that eliminates any parallel data decomposi-

tion artifacts from the stored data. This offered consistent performance and regular data access patterns.

The second generation is really an evolution of the first with HDF-5 adding parallel capabilities and NetCDF bifurcating into NetCDF4 [15] and PnetCDF [9] with PnetCDF almost completely maintaining the data model and NetCDF4 shifting to use HDF5 underneath. The other improvement is incorporating knowledge of an underlying parallel file system to support large files written in unision from many processes.

The third generation is a reaction to the second based on recognizing that maintaining the logical data model in physical form became inordinately expensive [10] and offered a performance penalty in most cases when running at scale. Libraries like ADIOS [11] shifted from writing complete variables from distributed processes as a single entity to treating all data from a single source to be treated as a unit. This eliminated the data reorganization at the cost of more complicated reading patterns. In spite of this extra complication, the performance is generally better [10].

SIRIUS represents the next generation. New platforms are introducing additional storage layers to accelerate IO operations and to compensate for plateauing storage array performance. At the same time, data sizes continue to grow. The fourth generation IO API will have to both address the IO API and middleware layer as well as the deeper, more complex storage hierarchy. SIRIUS considers the local portion of each globally distributed variable as a management entity with data placement decisions across the entire storage hierarchy rather than on a single tier. Decisions on what data to place where is driven by the data contents itself according to end-user specified priorities and system characteristics. For example, if temperature and pressure are nearly always retrieved together, organizing the data to keep just these two arrays together without any interleaving from other variables or scalars will accelerate later reading. If these variables could also be “processed” such that the important data

features are maintained in high resolution while less interesting regions are stored in highly compressed—even using lossy compression—forms, the amount of data written can be greatly increased. While accelerating writing is important. This approach also supports accelerating reading.

This paper presents an overview of the efforts to build such a fourth generation storage and IO system. A discussion of the platform features, storage challenges, quality of service features, and metadata challenges are all discussed briefly.

The rest of the paper is organized as follows. A brief overview of related work is presented first in Section 2. Section 3 discusses the differentiating platform features SIRIUS will provide. Section 4 discusses the challenges and opportunities for deploying scalable storage infrastructure. Section 5 discusses the quality of service features proposed for this project. Next is an exploration of the metadata challenges required to support such a system in Section 6. An initial prototype demonstration of the functionality is presented in Section 7. The paper is concluded in Section 8 with a summary of the broad issues covered in the paper.

2 Related Work

Ceph [18] is a distributed object store and file system. It offers both a POSIX and object interface including features typically found in parallel file systems. Ceph’s unique striping approach uses pseudo-random numbers with a known seed eliminating the need for the metadata service to track where each stripe in a parallel file is placed. PVFS [3] offers optimizations to reduce metadata server load, such as a single process opening a file and sharing the handle. It has been commercialized in recent years as OrangeFS. Lustre [2] has become the de facto standard on most major clusters offering scalable performance and fine-grained end-user and programmatic control over how data is placed in the storage system. GPFS [16] offers a hands-off approach for providing good performance for scaling parallel IO tasks and is used extensively by its owner, IBM. Panasas [12] seeks to offer a dynamically adaptive striping system that detects the need for additional stripes for performance and adjusts the file layout as necessary.

Other file systems, like GoogleFS [6] and HDFS [17], address distributed rather than parallel computing and cannot be compared directly. The primary difference between distributed and parallel file systems is the ability of the file system to store and retrieve data simultaneously from multiple clients, in parallel, and treat the resulting collection of pieces as a single object. Distributed file systems rely on a single client creating a file, but distributing the set of files across a wide array of storage de-

vices. The other, popular distributed file system of note is NFS [13] that has been used for decades for enterprise file systems.

3 Platform Features

The platform has two key features that drive the rest of the design. First is the data refactoring/compression approach. Second are quality of service estimates.

3.1 Refactoring

Refactoring may be a uniform operation across an entire variable. For example, splitting a double into three parts—two bytes, four bytes, and two bytes, yields a two-byte value that is the majority of the data precision. The next four bytes would be most of the rest of the data precision. The last two bytes are the remainder of the precision. For quick overviews, just reading the two-byte portion is sufficient to get a rough idea of data contents. If particular data looks interesting, more and more data can be read to improve the precision. This can easily be applied uniformly by each process without coordinating. From a storage hierarchy perspective, the primary value portion could be written to high performance, low capacity storage while the rest is written to slower storage. That would reduce the data quantity written to NVM, for example, by 75% for a 2/6 split enabling far more output to be written to this fast tier with the rest spooled asynchronously.

A similar approach that maintains full data quality is to use a data stride to store only a data subset. For example, by selecting every fourth element in three dimensions yields a $\frac{1}{64}$ sized data set to store in fast storage—a mere 1.5% of the original size. The rest can be spooled asynchronously. Combining byte-splits and striding can reduce the data sizes even more. Doing a 3/5 split and an every fourth element yields 0.9% of the original size.

A more complex, but interesting approach is to offer an *Auditor* that performs a similar, but lower precision computation that greatly reduces computation intensity with only a minor loss of precision over short spatial and temporal domains. As the simulation progresses, the auditor drift would need to be reset to bring it back into alignment. The much smaller, reduced precision data could be used instead of the full precision in many circumstances. For an example auditor, consider a previous generation physics model. While it is not as accurate as the state-of-the-art-model, it is very close, particularly over short temporal and spatial ranges. Other types of auditors are possible and are under investigation. The key idea with the auditor is that the reduced quality result can be calculated much more quickly than the full precision and will have much smaller data sizes. As a

side benefit, the auditor can both detect soft errors in the calculation by the drift from the high precision physics diverging too quickly. It can also be used to create a statistically representative data set for the high precision physics model. Calculating the auditor value and writing its output for checkpoint restart or initial analysis exploration can save time and leverage otherwise idle excess compute resources.

A more dynamic lossy approach would be to apply a wavelet compression [7] approach that generates different compressed data sizes at a fixed error rate depending on the data entropy. These are still uniform operators, but the resulting data can be of radically different sizes. For this approach, some or all of the lower precision data can be written to the fast tier while full precision can be spooled asynchronously to the slower tier(s).

A middle ground approach between these refactoring approaches is to use a non-uniform operator across a variable. Instead of, for example, splitting on byte boundaries to make multiple values, a function that identifies data features through a local analytics function could identify “interesting” data that should be maintained in full precision while other areas can be more highly compressed. Such an operator would decompose the data from a process further than a single process or node depending on the data features. This approach may balance precision better than wavelet compression, but at a higher analytics cost. SIRIUS would put data areas with interesting features on the fast tier while the rest could be spooled to the slow tier asynchronously.

We plan to investigate all of these approaches as different applications will have different techniques that work best. Our initial tests have demonstrated the potential for the auditor approach in an isolated environment. We have also built a prototype ADIOS transport method for the byte-split approach. Any performant storage system should offer the flexibility to incorporate application specific data refactoring techniques and sufficient metadata support for an arbitrary client to access the data successfully.

3.2 Quality of Service

Quality of service deadlines are important for driving how much time is spent performing IO. At the same time, data quality must be maintained at a sufficient level for the resulting science to be possible. The system must offer a way for an end-user to negotiate with the system for trading off between time spent in IO and the amount of data written or read. Part of that tradeoff will be increased or reduced data quality, depending on the system. For example, when data is written, a few different forms may be output given sufficient space and time. One may be every fourth element across a regular mesh

Table 1: Reading Options for Variable “A”

#	Size	Time	Time Err	Refactoring	Data Err
1	$(\frac{1}{4})^3(\frac{3}{8})A$	10s	$\pm 3s$	stride, byte-split	98%
2	$(\frac{3}{4})^3(\frac{3}{8})A$	90s	$\pm 30s$	stride, byte-split	58%
3	$(\frac{1}{4})^3(\frac{2}{8})A$	16s	$\pm 5s$	stride, byte-split	n/a
4	$(\frac{3}{4})^3(\frac{2}{8})A$	120s	$\pm 50s$	stride, byte-split	n/a
5	$(\frac{1}{4})^3A$	1200s	$\pm 30s$	stride	98%
6	$(\frac{3}{4})^3A$	2400s	$\pm 90s$	stride	58%
7	$(\frac{3}{8})A$	1350s	$\pm 120s$	byte-split	0.02%
8	$(\frac{2}{8})A$	2250s	$\pm 120s$	byte-split	n/a
9	A	36s	$\pm 6s$	wavelet	1%
10	A	3600s	$\pm 600s$	none	0%

reduces the data size to $1/64^{th}$ the full data set. Further dividing that using byte-splitting can reduce it by another 75%. For quick overviews to search data sets, this reduced form can be sufficient driving which data sets should be investigated in more detail. The key driving factor is time. The application scientist can read 0.4% of the full data volume with a similar time reduction. SIRIUS will offer a negotiation process to read any data.

The byte splitting approach error rate is quite small. By splitting at byte boundaries rather than converting to a lower precision 4-byte float, we preserve the full exponent range and keep the first 11 bits of mantissa precision. This leaves a 2^{-12} maximum error magnitude for each value—the last 40 bits represent less precision together than the immediately preceding bit all by itself.

To read these various data organizations, read operations will shift to a two-step process. First, an list of options will be requested that includes both and error estimates. A second request will retrieve a particular data portion from the provided list. Consider Table 1. First, a user will request a particular variable and timesetp. SIRIUS will return a table similar to Table 1. For a given variable “A”, the end-user can then select the data quality and approximate reading time for the operation. In this case, there are 5 options for obtaining the whole data set (1/2/3/4, 5/6, 7/8, 9, 10). The first four entries represent a spatial and byte split, 5/6 represent just strided writing, 7/8 represent just a byte-split, 9 represents a wavelet compressed version, and 10 is the full precision data. The user would specify to read a particular data instance that would proceed normally. Quality of Service soft guarantees specified as part of the request will result in SIRIUS allocating soft bandwidth reservations to meet the request. While some of the error rates seem to render the data unusable, consider a 3000x3000x3000 simulation domain. That would yield a 27 gigapixel image should all of the data be used. Visualization will already radically reduce the data sizes to make usable visualizations

that work on a standard display. A 99% reduction would yield a 270 megapixel image—still quite large.

4 Storage Challenges and Opportunities

The supercomputing platforms being deployed today are all incorporating a Non-volatile memory (NVM) layer as a fast cache between compute and the storage array. The assumption is that nearly all IO will be performed against this layer to hide the much greater latency to the storage array. The challenge is the NVM capacity is expensive limiting the amount deployed. The unspoken limitation is that this fast layer still must drain to the relatively slow storage array. This performance mismatch will limit capacity and performance just due to the drain and data stage-in operations.

A more effective way to use these resources is to only store the most important data in the fast tier and store lower precision representations of the rest of the data in the slower tiers. This lowers pressures on the NVM layer increasing performance overall by greatly reducing the drain/stage-in operations and reducing the data volumes stored on a per application basis. As part of the data refactoring, SIRIUS will use the entire storage hierarchy to store different portions of each variable as illustrated in Table 1. For example, for the 1/2/3/4 setup, 4 different tiers may be used to store this single variable.

5 Quality of Service Features

SIRIUS offers a novel feature related to managing IO time as a first class characteristic. Rather than being at the mercy of the storage array performance, an end-user can describe the local data to the storage system and receive an estimate on how long that data will take to write. If that is acceptable within a margin of error, the API can write. If it is unacceptable, the end-user can make decisions about skipping the output or maybe spending a little time with a strong data refactoring to reduce the data size. On reading, a user will select from a list of available options based on the time and data quality requirements.

Key to making QoS work is to maintain performance metadata to inform the IO time estimates and error bounds returned to the user. Without hard reservations, no system can offer strict performance guarantees. Instead, by monitoring system behavior, SIRIUS will be able to offer reasonable time estimates given data placement and the requesting source(s).

6 Metadata Challenges

The metadata system has a daunting challenge. Traditional metadata systems for both distributed and paral-

Table 2: Performance For 3/5 byte Split

Test	Time (s)
Write full data	10.3
Byte split	2.5
write 3-byte portion	3.4
write 5-byte portion	9.3
Read 3-byte portion	10.3
Reassemble after read	27.9
Read full data	34.2

lel file systems only have to deal with a single name space and storage tier. While hierarchical storage management [1] systems offer a way to show a single name space, the reality is that the tier closest to the user is a cache for the other tiers with data migrating as necessary to support user interaction. SIRIUS is working in a fundamentally different way. Each tier is treated as a first class citizen with direct client access possible. Where data is actually retrieved from is where it is actually stored rather than forcing data migration and caching. Systems like Sirocco [5] offer a way to support this model directly and are a fundamental part of our system.

The additional challenge SIRIUS metadata services face is incorporating user-specified attributes including data refactoring functions. Since an arbitrary user must be able to access any data written for which they have permissions. Having data locked behind data compression that has changed over time may result in effectively encrypting data and losing the decryption key.

We also seek to offer the ability to also store multiple versions of the same data using different refactoring techniques. This will offer additional options for higher precision OR higher performance reading.

7 Demonstration

Our initial tests are on the Sith cluster at Oak Ridge. The system contains 40 compute nodes. Each compute node contains four 2.3 GHz 8 core AMD Opteron processors, and 64 GB of memory. The system is configured with a 86 TB Lustre file system for scratch space.

We use the XGC1 [8] fusion simulation as our application. We run on 5 nodes with 160 processes total. XGC1 is configured to use 819,200,000 particles evenly spread across the processes. Performance numbers are presented in Table 2.

Evaluating the error when using just the 3-byte portion compared to the full data set yields an L^2 norm of 72028.2 and L_{inf} of 0.00109242.

Writing the 3-byte portion synchronously to fast storage and spooling the 5-byte portion out to slower storage

asynchronously will preserve the full data fidelity while improving both writing and reading time even when including the disassemble/reassemble times. The introduced errors when using just the 3-byte portion, as discussed above, is quite small.

8 Conclusions

Overall, the SIRIUS storage system is ushering in a new generation of both IO APIs and storage system managed together. It incorporates additional metadata to help accelerate data access and ultimately time to insight. Our initial efforts show promise that such a system is both possible and can offer attractive performance to better use the supercomputing platform. By treating all storage tiers as first-class resources accessed independently, SIRIUS can maximize available IO bandwidth. By refactoring data to extract out important parts into separate data set slices, data writing and reading time can be greatly improved while still maintaining full data fidelity when necessary. The quality of service monitoring will inform the performance estimates giving a more predictably responsive system accelerating time to insight.

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