Towards Exascale Scientific Metadata Management

Spyros Blanas
The Ohio State University
blanas.2@osu.edu

Surendra Byna
Lawrence Berkeley National Laboratory
sbyna@lbl.gov

Abstract

Advances in technology and computing hardware are enabling scientists from all areas of science to produce massive amounts of data using large-scale simulations or observational facilities. In this era of data deluge, effective coordination between the data production and the analysis phases hinges on the availability of metadata that describe the scientific datasets. Existing workflow engines have been capturing a limited form of metadata to provide provenance information about the identity and lineage of the data. However, much of the data produced by simulations, experiments, and analyses still need to be annotated manually in an ad hoc manner by domain scientists. Systematic and transparent acquisition of rich metadata becomes a crucial prerequisite to sustain and accelerate the pace of scientific innovation. Yet, ubiquitous and domain-agnostic metadata management infrastructure that can meet the demands of extreme-scale science is notable by its absence.

To address this gap in scientific data management research and practice, we present our vision for an integrated approach that (1) automatically captures and manipulates information-rich metadata while the data is being produced or analyzed and (2) stores metadata within each dataset to permeate metadata-oblivious processes and to query metadata through established and standardized data access interfaces. We motivate the need for the proposed integrated approach using applications from plasma physics, climate modeling and neuroscience, and then discuss research challenges and possible solutions.

1 Introduction

The observation or simulation of natural phenomena produces massive datasets that are cumbersome to manage. Although many efforts are underway to address the research challenges of storing and analyzing large scientific datasets, the research community has paid less attention in using domain-agnostic metadata to improve performance and scientific productivity. Metadata is essential to automate scientific analysis tasks and workflows, and can bring logical data independence to scientific applications through metadata-aware scientific management tools [18]. Information-rich metadata, such as low-resolution snapshots of datasets and of results from historical analyses, have the potential to guide scientists or runtimes to perform data analysis more efficiently. In addition, effective collaboration between teams frequently hinges on succinctly conveying the salient properties of a large dataset as metadata. Therefore, systematic management of information-rich metadata can be a catalyst for scientific productivity when progress depends on the coordination of hundreds of scientific teams that span discipline boundaries. For instance, understanding of the effects of global warming on future generations involves more than 1,200 scientists in the IPCC's AR-5 Working Group II alone [23]. Unfortunately, the vision of systematic scientific metadata management across heterogeneous analysis tools and science disciplines largely remains unrealized.

Conventional practice for scientific metadata management varies between scientific domains, and sometimes even between individual applications. The scientific metadata that are collected today can be classified in three broad categories. *Descriptive metadata* are integrated within datasets and are largely tailored to help scientists locate and read data variables. Even file format libraries and systems that are designed for large-scale scientific data analysis such as ADIOS/BP [1] and SciDB [40] store little metadata beyond quantile information for each block of data. Metadata conveyed in *ad-hoc text annotations* have high information density but are time-consuming to generate. Because of this productivity cost, datasets are selectively annotated with ad-hoc information during data curation. An unfortunate consequence is that many datasets

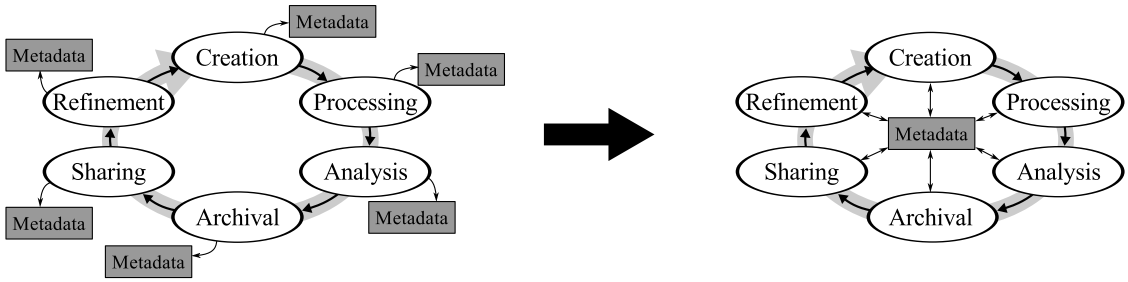

Figure 1: Our vision for exascale scientific metadata management integrates metadata information currently in disparate containers into a single metadata acquisition and storage framework that integrates with established scientific file formats.

that scientists interact with daily are in intermediate, non-curated forms without any metadata annotations. *Data provenance* metadata is automatically captured by workflow systems and reveals information about the data generating process, any data transformations, the historical analyses and their associated data movement. However, data movement that is oblivious to the workflow system (such as a file transfer) severs the connection between a dataset and its provenance metadata because of their physical separation in different storage locations.

Existing metadata management practices prove insufficient when analyzing massive datasets using tens of thousands of CPU cores at leadership computing facilities. At this compute scale and data volume, scientists require guidance on how to perform data triage and decide what dataset fragments need to be processed first or ignored. Data analysis runtimes rely on external information from an infrastructure expert to tune parallel I/O and optimally co-locate dataset fragments that are analyzed simultaneously. Data curators have to manually discover what metadata are available for each dataset and data variable to verify whether it is accurate or outdated. We posit that scientific metadata ought to be captured automatically, stored within the scientific dataset, and be accessed as frictionlessly as regular data to quicken the pace of scientific discovery. Our investigation is motivated by two questions:

- What new metadata types can be captured systematically that will accelerate scientific discovery?
- How can this metadata be acquired, stored, and queried efficiently?

In this paper, we categorize existing metadata management practices, discuss use cases for information-rich metadata for accelerating representative scientific applications and present some research challenges in realizing this vision. We elaborate on the current practices for managing metadata and discuss the potential of integrated metadata management to impact the data-driven discovery process in Section 2. We motivate the need for automated metadata acquisition and management using scientific applications from plasma physics, climate modeling and analysis, and neuroscience in Section 3. We discuss research challenges and possible solutions in acquiring, storing and accessing rich metadata in Section 4. We discuss related work in Section 5 and conclude the paper in Section 6.

2 A vision for integrated metadata management

2.1 Metadata and data-driven discovery

Data-driven scientific discovery often follows a cyclical pattern of data creation, processing, analysis, archival, and sharing [47]. The shared dataset then becomes the seed for follow-up investigations that further refine the research question or investigate new hypotheses. This triggers the start of another iteration of the cycle. Although metadata are generated and consumed in every step of this cycle, the management of this metadata information across different phases is unprincipled (shown on the left in Figure 1). A metadata management framework for extreme-scale science needs to capture metadata during all phases of the data life cycle and expose that information to data generation or analysis tasks. This is shown on the right in Figure 1.

We envision an integrated metadata management framework that augments scientific data with information that (1) is semantically richer, (2) is stored within each dataset and can be accessed via established data access and querying interfaces, and (3) is acquired, propagated, and managed automatically. Richer metadata become a necessity because the cost of sifting through an entire dataset to extract a particular property of the data grows exponentially compared to the cost of storing and transferring this property as metadata. By storing metadata within a dataset, metadata can seamlessly propagate through file-centric analyses and be easily transferred to other scientists or computing facilities. By relying on established data access interfaces for metadata access and storage, next-generation scientific metadata management is unfettered from particular analysis tools or workflow engines.

We identify four critical roles for information-rich metadata in the data-driven scientific discovery cycle: Metadata can be used to appraise a new dataset or acquaint a scientist with a curated dataset, develop, and deploy a meaningful analysis, acquire insights and propagate them across analysis, and accelerate data curation. We now elaborate on these four roles.

Appraise and acquaint with a dataset

In the first phase of the cycle, a scientist is given access to an interesting dataset and uses metadata to acquaint himself with the dataset and appraise its scientific value. Currently, datasets embed a limited form of metadata, such as a list of the data objects that the dataset consists of, schema information, and the shape and dimensionality of each data object. This metadata information is commonly insufficient, and additional insights are derived by computing simple statistics on particular data objects and/or selectively visualizing data fragments of interest. In addition, scientists communicate with the data producer(s) for additional information about the dataset. Collectively, the information contained in these summarizations, visualizations, e-mails and meeting notes semantically annotates the dataset.

Exascale science requires richer metadata that is embedded within scientific datasets. An information-rich metadata management framework should allow scientists to understand a dataset through multi-resolution summaries that have been retained from prior analyses and are embedded in the data. Metadata-aware analysis tools can leverage multi-resolution summaries and accelerate exploratory data analysis. The summaries of the datasets from prior analyses can be visualized instantly. This substantially increases the scientific re-use value of the dataset.

Develop and deploy analyses

After the salient properties of the dataset are extracted, the scientist decides on the appropriate domain-specific analysis that will be performed and starts collecting the tools or developing the code to perform the analysis with tens of thousands of CPU cores. Scientists need to debug and verify the output of an analysis using a small representative sample of the dataset. In this process, the scientist manually specifies additional metadata that is specific to the dataset (such as what is a meaningful sample for verification) and to the analysis infrastructure (such as particular file locations or the available memory per node). Larger and larger dataset samples are analyzed and verified, until there is confidence that this analysis is correct and well-tuned for a production run.

The proposed integrated scientific metadata framework shall retain information on what analyses have been previously evaluated on a dataset. The framework shall store qualitative information that is specific to each analysis, such as dataset access patterns and access correlations across datasets. In addition, the framework has to capture the observed I/O and CPU performance, as well as hardware configuration details, such as number of CPU cores used, memory, parallel file system configuration, computer topology, etc. Richer metadata information about an analysis and its execution environment allows scientists to spend less time debugging and tuning large-scale data processing pipelines. During deployment, scientific tools can use the performance data stored as metadata to further optimize and refine how an analysis will be executed.

Acquire and propagate insights

If the analysis is orchestrated using a workflow system, provenance information is automatically captured in a separate data store, which may be a relational database management system. Existing systems such as MPO (Metadata, Provenance, and Ontology) [52] is an example of this approach. The representation and storage of provenance information is specific to the workflow system used by the scientist. Otherwise, the

		Metadata storage	
		Segregated	**Integrated**
Metadata source	**Human-generated**	Ad-hoc annotations	List of data objects Array dimensionality and shape Schema and chunking information
	Automatically acquired	Provenance	Multi-resolution summaries Access patterns Observed performance Cross-dataset correlations Audit log of modifications

Table 1: Classification of metadata based on who provides/acquires metadata and where metadata is stored. Human-generated metadata is acquired using ad-hoc annotations stored either in 'readme.txt' files, scientists' logbooks, etc., and using high-level I/O libraries such as HDF5, NetCDF, and ADIOS. Workflow systems acquire provenance related metadata automatically. Our vision for rich metadata, such as summaries, data usage patterns, performance, etc. is highlighted to acquire automatically.

scientist must manually acquire, manage and propagate metadata information using scripts to a metadata-aware analysis task. Tasks access metadata information via a proprietary interface that is specific to the storage layout and representation of the metadata.

Our vision is to embed sophisticated metadata acquisition and management primitives within popular scientific file formats. Thus, current applications will automatically capture information-rich metadata, such as cross-dataset correlations, without modifying existing analysis tools. Scientific metadata are stored within the dataset and are managed by the file format library. Metadata can then be accessed through the same established access interfaces for regular data objects.

Curate data

The curation process aims to preserve selected datasets and their metadata for reuse. Curation is commonly performed manually and selectively by the domain expert. The first step is to discard data that will not be curated, and transform the dataset to a format that is appropriate for long-term storage. This metadata-oblivious transformation inadvertently strips datasets from all but the most essential metadata (such as variable type information). Metadata information that is stored separately, such as lineage information from a workflow system, becomes stale. Currently, the last step of the curation process augments the curated dataset with semantically richer metadata information that the domain expert deems necessary for future analyses. Such metadata are commonly curated as ad-hoc annotations to the dataset.

With our vision of embedding metadata within the dataset, metadata curation becomes an integral and concurrent part of the data curation process. Automatically acquiring, managing, and propagating metadata within existing analysis pipelines will produce metadata-rich datasets with minimal involvement from domain experts, which can thus relieve the need for extensive ad-hoc metadata annotations during data curation. We anticipate that transparent metadata acquisition and management will make scientists more likely to consume, produce, and share metadata-rich datasets. This expectation is supported by anecdotal evidence that scientists become more reluctant to share datasets as the metadata annotation requirements become more onerous [12].

Scientists can use the curated access metadata to reconstruct an audit trail of accesses to the dataset and understand what portions of the data other scientists have analyzed extensively, and what analyses have been performed. Infrastructure providers of supercomputing systems can use performance-related aspects of curated metadata to make informed procurement and deployment decisions. The broader scientific community and the general public can use information about dataset and fragment popularity to identify influential datasets, data providers and projects, and acknowledge their role in advancing large-scale data-driven science.

2.2 A classification of metadata information

From our interactions with scientists across different domains, we have observed that there is substantial diversity in the metadata information that scientists interact with. In Table 1, we show a classification of metadata types based on who provides metadata and where metadata is stored. The common metadata acquisition sources are scientists or application developers (labeled as 'Human-generated') and software libraries and tools ('Automatically acquired'). Metadata is often stored within the data files (labeled as 'Integrated') or in separate files or database systems ('Segregated'). We briefly discuss these categories in the following paragraphs.

User-defined metadata prior to data generation: Starting from the top right corner in Table 1, some metadata are provided explicitly by a scientist at the moment of data production. Examples include data type and endianness information, or the dimensionality and chunking strategy of an array for defining the layout of data on a disk. Under this paradigm, a particular file format, such as HDF5, or data encoding defines the collected metadata in advance and stores the metadata within the dataset. For example, in HDF5 file format [45], metadata is stored as the attributes of the file. Existing file format libraries already provide support to capture and propagate this type of metadata; otherwise the dataset would be indecipherable for analysis.

Ad-hoc metadata that annotate a dataset: Another way to acquire metadata is to explicitly request it by the domain expert. Many times, however, important information that describes specific features or properties of the data cannot be shoehorned into this rigid format. Scientists describe these properties in plain text that accompanies the dataset. As shown in the top left corner in Table 1, such metadata can be logically thought as an annotation to an existing dataset which is stored separately from the data. Common techniques that use this metadata management paradigm include publishing `readme.txt` files at the same website or file system folder as the dataset, as well as electronic or face-to-face communication. In certain instances this form of metadata is captured in the logbooks of scientists and can only be acquired through direct communication.

Workflow-based metadata: Several scientific workflow systems are in use to automate task coordination and management in complex workflows. Workflow systems collect information that is mainly related to the provenance of the data and is used to quickly identify (or repeat) the process that generated a specific fragment of a dataset. Each workflow system stores and manages provenance metadata differently, and no standardized interface to access lineage information from applications currently exists. Should a scientist desire to access the provenance metadata, they first need to learn the data model and the query interface of the workflow system. Some workflow systems store provenance metadata in a relational database and scientists can query the database using SQL [52]. Other systems use representations that are optimized for provenance metadata, and scientists query provenance metadata through a system-specific API [25].

Towards information-rich metadata

In the extreme-scale data era that many scientific domains are entering, it becomes necessary to automatically collect information-rich metadata that go beyond provenance. Rich metadata include multi-resolution snapshots of data, summarizations, and semantic relationships among datasets. We classify the new types of metadata that can be automatically captured in five broad categories:

1. **Identity information** includes the dataset name or any other unique identifier, the application producing the dataset, and reproducibility information such as the task and its parameters that were used to produce the result.
2. **Dataset descriptions** include summary statistics, derived variables, the resolution of the dataset, and the location of low-resolution snapshots of data for quick visualizations.
3. **Performance and profiling information** are historical access patterns, the presence of augmented datasets (such as indexes, partial replicas, or materialized views), and the locations of physically reorganized layouts of the data for faster access. This category also includes prior response time and energy consumption measurements that can be used for optimization decisions. This information can be readily leveraged for exploratory scientific data analysis [49].
4. **Relationships** among various datasets or tasks, such as derived variables of a dataset, or possible computations to derive such a variable upon request. This includes information on different views of

the same dataset, such as a sorted replica or a bitmap index. Relationship metadata captures how analysis results are computed and where the results are stored.

5. **User-defined metadata.** Users and applications will be able to specify additional metadata to extend the semantic information conveyed as metadata.

3 Science drivers

The proposed vision for integrated metadata management is useful for a wide variety of scientific applications. In this section, we use applications from plasma physics, climate modeling and neuroscience to motivate the need and the potential benefits of information-rich metadata.

3.1 Plasma Physics

Scientific simulations in various fields of physics use large-scale supercomputers for understanding the phenomena that affect our universe. Collisionless magnetic reconnection is one such important phenomenon that releases energy explosively as magnetic field lines break and reconnect in plasmas. This is a mechanism responsible for the aurora when the Earth's magnetosphere reacts to solar eruptions. Magnetic reconnection is initiated in the small scale around individual electrons but eventually leads to a large-scale reconfiguration of the magnetic field. Recent simulations [48] have revealed that electron kinetic physics is not only important in triggering reconnection, but also in its subsequent evolution.

Fueled by new capabilities of highly-optimized simulations, large-scale computers have been providing the first glimpses of various physics phenomenon in a high resolution and multidimensional space. The amount of data produced by these simulations is massive. For instance, a recent execution of the VPIC simulation on 120,000 CPU cores of the Hopper supercomputing system at the National Energy Research Scientific Computing Center (NERSC) produced 400 TB of data. Yet, this massive amount of data corresponds to only 10 out of the 23,000 simulated time steps! To counter the data volume problem, scientists often perform various analyses while the data is in memory and discard intermediate data. This analysis process is called *in situ* and is sometimes used for reducing the amount of data to be stored. The complete particle dataset will be processed and stored for only one or two final time steps instead. The burden of managing and orchestrating the *in situ* analyses, however, lies with the scientists that use existing processing libraries, such as ADIOS [1] and Glean [17]. The absence of standardized metadata management is an obstacle to automated coordination and synthesis of multiple discrete *in situ* analyses.

Complicating the picture further, these *in situ* analyses will need to be continuously maintained and augmented to be conscious to future changes in the memory and storage hierarchy. Upcoming extreme-scale architectures will likely include technologies such as large main memory, non-volatile memory, and flash-based storage in the form of burst buffers for simulation and staging nodes. Making use of these memory and storage resources is necessary for energy efficiency and high performance. Storing metadata regarding optimizations previously applied in improving these massive data I/O and results from previous analysis will benefit not only performance, but also scientific productivity.

3.2 Climate Modeling and Analysis

Efficient collaboration among climate scientists is critical in accelerating the understanding of the effects of climate change on future generations. The number of scientists involved in climate modeling and analysis is enormous. For example, there are more than 1,200 scientists in the IPCC's AR-5 Working Group II alone [23]. Climate research has a long history of heavily relying on metadata to interpret scientific observations. The climate research community has embraced self-describing and machine-independent data formats, and the netCDF data format [38] in particular is widely accepted for disseminating scientific datasets.

Multiple standardization efforts exist to encourage the exchange of climate data observations and analyses. The National Oceanic and Atmospheric Administration has proposed the Cooperative Ocean/Atmosphere Research Data Service (COARDS) [11] conventions to encourage the standardization of the metadata for global atmospheric and oceanographic research data sets. The Program For Climate Model Diagnosis and Intercomparison (PCMDI), that manages the CMIP3 and CMIP5 model data has proposed the Climate and Forecast (CF) Metadata Convention to generalize and extend the COARDS conventions for datasets that use the netCDF API [35]. In a similar effort, the Numerical Model Metadata (NMM) initiative [32] has standardized the description of the numerical model used to produce climate data. This includes information such as a formal and comprehensive description of the model and the parameter settings used to run the model. Other efforts have provided interfaces to annotate datasets with particular types of metadata. These include the Earth System Modeling Framework (ESMF) [15], the PRogram for Integrated earth System Modeling (PRISM) [36], and the Earth System Grid (ESG) [14]. To encourage meta-analysis and synthesis studies, the Earth System Curator [13] proposed a metadata infrastructure that combines and curates metadata from commonly-used packages for climate modeling.

Despite these standardization efforts, extensive user involvement is needed to add metadata and provenance information. In addition, the quality and type of metadata that are provided depends entirely on the scientists and the conventions of the organizations that provide the data. For example, in the CMIP5 datasets, the variance in the number of days reported per year is diverse. Some models uniformly use 30 days for every month, which amounts to 360 days per year. Other models represent the number of days in each month accurately, but omit a leap day in February to simplify year-over-year analyses, which results every year in a dataset having exactly 365 days. In the meantime, raw observation data from sensors commonly handle leap years correctly. While all these models use the same conventions to store the metadata, climate data analysis scientists still have to adjust and tune their analysis applications based on their understanding of these conventions. Multiple other incompatibilities exist that burden climate data scientists further. As a consequence, many climate research datasets are annotated selectively after the analysis has determined that the findings have sufficient scientific significance to merit the additional effort.

Similar to the VPIC magnetic reconnection application, climate simulations also can take advantage of *in situ* analysis. For instance, climate model simulations write data to disk in periodic intervals. Extreme events, such as tornados, may quickly form and then disappear before writing a snapshot of the simulation to disk. Interesting features between those intervals may be lost, and increasing the frequency of the writes may be impractical. These events can be detected dynamically through *in situ* analyses. Storing and managing metadata of these in situ detections for further inspection will improve the quality of data significantly.

3.3 Neuroscience

Recent initiatives to better understand the human brain [3, 5] have spawned research efforts that collect enormous amounts of neuroscience data. The sources of neuroimaging data span a wide variety of instruments and techniques including computed tomography (CT), diffuse optical imaging (DOI), magnetic resonance imaging (MRI), functional magnetic resonance imaging (fMRI), Positron emission tomography (PET), etc. These instruments produce data in different formats depending on their manufacturer. In addition, metadata corresponding to each data set examining the same subject or sample are highly likely to be different as well. In this scenario, extracting and managing relationships among different images of the same subject/sample is a critical requirement to improve the understanding of neuroscience data. We are not, however, aware of any proposal to automatically extract and manage relationships among scientific datasets in a systematic manner.

After the extraction of metadata and their relationships, the requirement of searching them is another challenge. Several solutions targeting bio-medical imaging specifically have been proposed [27, 20]. Systems such as MPO [52], the SPOT suite [44], the JGI Archive and Metadata Organizer [24], and ESGF [14] have been actively providing metadata search capabilities. While the data remains in these systems, searching data and metadata is possible. However, once the data is outside these systems, searching metadata becomes cumbersome. In fact, in many cases the metadata of interest may not be stored within the data file. To search the metadata, scientists have to develop custom solutions for accessing these external metadata sources. A requirement for a metadata management framework is to portably manage metadata and support movement, extraction, and search capabilities.

4 Research Challenges

The implementation of an integrated metadata management framework to support various types of scientific analyses faces several fundamental challenges that span the acquisition, storage, and access of metadata information. In this section we describe some foreseeable challenges and elaborate on possible solutions, in response to the following research questions:

1. What metadata has to be captured to make *in situ* and post-processing analyses more efficient? How does one collect metadata non-intrusively from different sources?
2. How should one store the collected metadata and provenance for efficient access? How can one control the storage space of information-rich metadata to ensure that the size of the dataset remains manageable?
3. How does one keep the metadata consistent and resilient in the presence of failures? How can one keep the metadata secure and control every access?

4.1 Acquiring metadata

4.1.1 Integrating automatic metadata acquisition into existing infrastructure

Collecting a comprehensive set of metadata requires tapping into multiple sources. The research challenge is identifying the appropriate component of the infrastructure stack to acquire the metadata of interest. Although it is easier to glean information-rich metadata from components that users directly interact with, such as analysis or visualization tools, this ecosystem is very diverse and segmented per scientific discipline. Low-level components of the stack, such as the file system or operating system, are ubiquitous among large-scale computing facilities but the acquired metadata may not have enough semantic information to be useful. We identify four abstract levels to intercept and acquire metadata for scientific applications:

1. **Analysis level:** Observing metadata information at the application level allows the framework to capture high-level information such as the analysis intent. Because of the diversity of the modern scientific toolbox among different scientific disciplines, acquiring high-level metadata requires user involvement. Commonly, the domain expert will express concepts and relationships using an established knowledge ontology, which may impede the productivity of non-experts users of the data.
2. **Library level:** Scientific analyses are rarely building every component from scratch; they instead rely on a common set of libraries to provide some core functionality. Examples of such libraries include BLAS for linear algebra, MPI for parallelization, and SQL connectors for issuing queries against a database. A metadata management framework could integrate with these libraries and transparently acquire metadata. The metadata information at this level is commonly rich in semantics (for instance, a BLAS function call translates to a single linear algebra operation), is high-level (for instance, a SQL query specifies what data should be returned, and not how they will be processed) and contains valuable details about the execution environment (for instance, instrumenting the MPI library can provide a wealth of metadata information on parallelization granularity and communication patterns). The challenge is that metadata information acquired at the library level will be partial and fragmented because only a limited number of libraries can be augmented with metadata acquisition capabilities.
3. **File format level:** Looking further away from the user, one finds that data resides in binary file formats following established specifications to maximize sharing and reuse. File formats such as netCDF, HDF5, ADIOS BP or SAM/BAM are *de facto* standards for data exchange among certain scientific communities. As all I/O is issued against a well-defined API that is specific to each file format library, a metadata management framework could conceivably glean metadata information from access requests that are directed towards the library. Some libraries, such as HDF5, are supporting this functionality natively through a virtual object layer (VOL) abstraction [8]. Metadata acquisition libraries that dynamically instrument codes can support other libraries such as POSIX-IO. An advantage of this technique is that metadata is acquired automatically without recompiling existing programs. The disadvantage is that data access requests at the file format level are imperative and stripped of semantic meaning, as requests retrieve specific columns of a table or cells in an array. Another drawback is that certain file formats, such as FITS or CSV files are not amenable to automated metadata acquisition as they lack an established programming interface to access data.
4. **Operating/file system level:** A metadata framework can also tap into the mature APIs that are available by the file system and the operating system. In addition to tracing system calls (for instance,

using `strace`), a framework can also observe detailed hardware performance counters and process statistics. Identity metadata information can be gathered from the process information and the computational infrastructure that is known to the operating system. The appeal of such a mechanism is that all analysis tasks can be observed without any code modification or involvement by the domain expert. However, at this layer only physical actions on byte streams can be observed. Logically equivalent actions that change the encoding but not the actual data (such as converting temperature from Celsius to Fahrenheit) cannot be readily identified at this level.

4.1.2 Discovering relationships between datasets

A significant research challenge is in capturing cross-dataset relationships and correlations as metadata. Analysis tasks today require manual orchestration by domain experts to fully exploit these relationships among data objects. The first cross-dataset property of interest is whether two or more datasets correspond to similar physical observations, yet are treated as separate datasets because of nuances of the data production process. An example of this type of cross-dataset relationship commonly arises in neuroscience, when analyzing a single brain specimen with two different instruments results in two files in different proprietary formats that scientists need to then analyze jointly and treat as a single dataset. Another cross-dataset property of interest is derived variables that require the concurrent analysis of different datasets. For example, relating pressure with wind velocity in a climate dataset for a particular geographical area may involve accessing data objects with different resolutions, that are produced by teams following different conventions and are stored in different file formats.

Capturing relationships among different datasets can be a semi-automatic approach. This may need some involvement from scientists in defining the basic mapping of variables. After the mappings are defined, during data production and analysis phases, runtime libraries can be used to extract the metadata information.

4.2 Storing and accessing metadata

4.2.1 Embedding metadata into datasets

The cornerstone of our vision for scientific metadata management is that metadata needs to be stored within datasets to prevent metadata-oblivious processes from destroying metadata information. This will accelerate the transition towards metadata-rich scientific processing pipelines.

Many scientific datasets are encoded in file formats that allow multiple data objects to be stored within a file. Embedding information-rich metadata objects in these file formats will require devising new object hierarchies for metadata. This requires metadata information to be discovered, encoded and accessed using the established interfaces of the underlying file format.

1. **Metadata discovery:** By embedding metadata within the data object hierarchy of a file format, metadata discovery needs to build on and extend existing data object discovery mechanisms. Metadata information, however, that masquerades as a regular data object may be accessed continuously during an analysis. Metadata discovery includes querying about the existence of a particular metadata class ("is there a summary of this dataset?") and navigating between metadata objects ("switch to a low-resolution summary for this analysis"). Popular file format libraries are implemented with the assumption that data object discovery is a rare event, as it occurs only at the beginning of the analysis. In addition, object-to-object navigation commonly requires node-to-node hops within tree-based hierarchies. More efficient metadata discovery and navigation mechanisms need to be designed for existing file format libraries to efficiently support exascale metadata-rich applications.
2. **Metadata encoding:** Scientific file formats are commonly designed around array-centric data models. Some metadata types such as multi-resolution summaries are naturally represented as arrays. Metadata information needs to be encoded in array-like objects in order to embed richer metadata within scientific file formats. The open research challenge is to devise efficient representations for different metadata classes, such as audit logs, that may lack a well-defined structure.
3. **Metadata access:** Scientific metadata information that is stored within scientific file formats is indistinguishable from regular data objects. The advantage to applications is that they can access metadata using the established data access interface. This interface, however, needs to be augmented to expose

the concurrency that will be available at both the cluster level and the node level in future computing infrastructure. (For instance VPIC, the magnetic reconnection simulation described in Section 3.1, already uses 120,000 CPU cores and is likely to approach the one-million-core scale in the future.) Existing data access mechanisms rely on data structures and communication patterns that are inherently non-scalable. A promising research direction is to investigate and resolve the scalability challenges that will allow metadata access interfaces to sustain the rate and volume of metadata requests that will be triggered by extreme-scale computing infrastructure.

4.2.2 Transactional semantics for metadata

Although file format libraries are designed to handle concurrent data operations, the correctness semantics of concurrent modifications are rarely described in the documentation. This is in part due to the complexity of describing what correctness means for all underlying components of the software stack, down to the operating system and the file system. This has not been a major concern for scientists so far because large-scale analyses are data-parallel and rarely update existing data. The append-only I/O pattern does not cause conflicts, and data partitioning isolates any infrequent updates to existing data objects. Unfortunately, metadata are shared by all tasks that operate on a dataset and will be continuously updated with new information.

A metadata management framework for scientific data needs to understand and expose the correctness semantics of concurrent metadata modifications to a scientist. Resilient systems rely on the notion of *transactional data operations* for this purpose. A transactional interface gives applications a consistent view of the metadata, and allows metadata modifications in complete isolation. This significantly simplifies the application logic, and allows the metadata management framework to perform sophisticated and holistic optimizations to an entire batch of metadata operations for efficiency.

Defining a transactional interface for metadata management leads to research questions about the foundations of transaction processing and concurrency control [19, 51]. The tuple-centric concurrency model of relational database systems is not sufficient for information-rich metadata objects. The first fundamental question is what is the unit of concurrency for rich metadata information. The second fundamental question is what is the set of permissible actions on the unit of concurrency, and what are their associated actions under the do/undo/redo protocol that will permit metadata operations to revert their effects. This naturally leads to the question of what does it mean for two transactional operations to conflict when updating metadata. What is an acceptable conflict resolution depends on the type of the metadata information and the scientific use case: conflicts in the dataset description or identity information may be intolerable as they can render a dataset inaccessible, but update conflicts in the data access pattern profile may be permissible if this information is only used for runtime optimization.

Controlling concurrent operations on metadata requires revisiting the fundamental techniques of *single-version locking* and *multi-versioning* and extending them for scientific metadata management. Synchronizing concurrent modifications via locking has high overhead, but always retains and returns the single latest version of metadata information. By design, multi-version concurrency control (MVCC) does not destroy or alter the original metadata when an application updates the metadata; the edit is applied to a new copy of the data instead. Retaining multiple versions can improve performance by redirecting reads and update requests to a different copy of the data [28]. In addition, when scientists wish to inspect older versions of a dataset, prior versions of metadata can be leveraged for answers. (This feature has been referred to as "time travel" querying in prior work [42].) Although reading a historic version does not violate the transactional semantics, it is unclear if this is desirable by scientific applications that act on the metadata information. Appropriate interfaces need to be developed to allow domain experts to specify their metadata freshness requirements for different types of metadata and different scientific analyses.

4.2.3 Storage size considerations

A metadata management framework also needs to determine what metadata should be discarded and when. One trivial solution would be to tie the life cycle of metadata to the life cycle of the associated data object: metadata collection starts when a data object is first created, and metadata are discarded when an object is deleted. However, there may be applications, such as security auditing, where it is necessary to preserve metadata even after the data has been discarded. The relative importance of different metadata information is only known by the domain expert. We therefore envision a scientific metadata management framework that allows a domain expert to specify a user-defined threshold per metadata class that is expressed as a fraction of the size of the base dataset. If the metadata size approaches the user-defined threshold, a metadata management framework can explore a number of options to reduce the storage footprint of the collected metadata.

1. **Selective disposal of metadata information:** One alternative to reduce the storage size of metadata information to is to selectively dispose metadata information. However, not all metadata information is equally valuable. It is thus natural to decompose this task into two orthogonal decisions: First, the framework needs to decide on the class of metadata that will be the "victim" for metadata disposal. The domain scientist can protect a class of metadata information through a `NEVER` directive, or indicate a strong preference to truncate metadata information from a particular class using an `ALWAYS` directive. Second, the framework needs to decide the metadata information from the "victim" class that will be discarded. The historical metadata access pattern could be used to identify infrequently used metadata and guide the decision.

2. **Semantic compaction of metadata information:**

   Another alternative is to semantically compact metadata to increase its information density. One form of compaction is entry consolidation: for example, an audit log that tracks accesses to individual array cells can cluster these accesses and express them as one access range. Compaction can also be achieved by computing metadata information on the fly from existing metadata. An example would be generating summaries at a desired resolution by summarizing higher-resolution datasets or through linear interpolation of lower-resolution datasets.

3. **Metadata-aware deduplication:** Future exascale systems will process massive scientific datasets. Because it will be very time-consuming to transfer datasets of this volume across computing facilities, data will be predominantly analyzed in the facility where they are stored. In this scenario, it will not be uncommon to find multiple copies of a dataset in a large-scale computing facility, often with minor differences, in the project directories of different teams. This exascale collaboration pattern presents an opportunity to leverage dataset similarities for automatic metadata-aware deduplication in the file system layer. These techniques extend the block-based approaches that are automatically applied by storage subsystems today and differ in that they will deduplicate at the logical (data) level, and not at the physical (byte) level. To effectively support logical deduplication, an exascale scientific metadata management framework needs to determine dataset lineage based on metadata. The research challenge is to develop efficient metadata-aware *diff* and *merge* algorithms that can quantify the lineage confidence between different datasets based on their metadata information. In addition, approximate algorithms must be developed that rely on incomplete metadata information to accommodate different metadata acquisition and metadata disposal practices.

4.2.4 Resilience and metadata consistency

As scientific applications like magnetic reconnection simulation approach the million-core scale, a single node failure becomes nearly certain. Although hardware failures remain relatively rare occurrences in supercomputers today, they are widely anticipated to become more common in future extreme-scale computing infrastructure. Analyses will be also interrupted for more mundane reasons, such as software bugs or transient communication failures. Workflow management systems can selectively repeat an analysis after failure, but rely on metadata to decide what tasks need to be restarted. Therefore, the consistency of the metadata information after a failure remains of paramount importance.

A key design goal of our metadata management solution is to tolerate and recover from hardware, software, or user errors graciously and systematically. A naïve solution to achieve durability is to store all metadata on a non-volatile storage medium, such as a hard disk, and write to this medium on every modification. The unprecedented concurrency of emerging scientific workloads will trigger millions of minuscule metadata modifications per second. Although the metadata information is safe in a case of a failure, waiting for the data to reach stable storage on every update has three major drawbacks: (1) it increases the response time for every metadata modification, (2) it is energy inefficient, as it cannot take advantage of caching, and (3) it drastically reduces the usable lifetime of modern non-volatile storage media like SSDs that support a limited number of write-erase cycles per cell. A metadata management framework needs to adapt write-ahead logging for the demands of extreme-scale applications, and evaluate high-availability techniques that are based on replication in a supercomputing environment.

4.2.5 In-memory metadata caching

A scientific metadata framework needs to provide capabilities to search metadata efficiently. Existing systems such as ESGF [14] and JAMO [24] provide searching metadata based on text, where the amount of metadata is minimal. Searching for extensive and information-rich metadata such as data summaries or performance metadata, requires an efficient storage organization of the information. Passively storing and retrieving metadata from disk-based storage, which has been the current practice for metadata management in workflow systems, will be prohibitively slow for emerging scientific use cases such as interactive scientific data visualization and real-time data analytics. Poor performance will be exacerbated by the unpredictable remote disk access latency in large-scale computing environments. Future metadata management frameworks will need to optimize metadata storage for low access latency. It is possible to achieve this goal using transparent architecture-conscious metadata placement in the memory and disk storage hierarchy.

The increasing degree of parallelism of future supercomputers will require novel storage techniques for metadata management. One can reasonably expect that applications will reserve the majority of the memory for scientific data analysis or simulation, and only a sliver of memory will be available for other information, such as metadata. Given the severe memory constraints, a promising research direction is to study data placement mechanisms and policies for metadata. We bring attention to three aspects of this problem:

1. Given an analysis or simulation task and its configuration parameters, what is the most relevant metadata to speed up the scientific discovery process?
2. When should the relevant metadata be retrieved from non-volatile storage and on what node should they be placed?
3. When should metadata be evicted from memory, and where should they be stored in the non-volatile storage hierarchy?

A light-weight prediction model can be used to identify the relevance of each metadata object for processing, depending on the type of the task and the data fragment it is processing. The model can leverage prior statistical knowledge of metadata accesses for smart metadata placement and prefetching. Novel hardware primitives such as hardware transactional memory, can further simplify application logic and improve performance [46].

4.2.6 Metadata confidentiality and access control

Even if a scientific dataset is publicly available, the metadata pertaining to this dataset must be carefully disseminated by the metadata management framework. Metadata information that relates to the production of the data and its processing would inadvertently disclose information about the data production process, which may be confidential. Relationship metadata and multi-resolution summaries of a public dataset may reveal the existence of related but confidential datasets, while stored performance profiles may disclose confidential infrastructural capabilities. If scientific metadata management is to become systematic and ubiquitous, a framework must guarantee *confidentiality* for metadata at rest, and *access control* to metadata in motion.

One research challenge is to develop a security model for metadata at rest. This model would rigorously define metadata information leakage and identify specific risk vectors. Based on this model, the user will specify non-permissible metadata information that will be discarded during acquisition based on the sensitivity of the analysis or the dataset. Assymetric cryptography of the metadata at rest can prevent metadata leakage if media theft occurs. In addition, the scientific metadata management framework needs to provide tools for selectively scrubbing sensitive metadata from datasets during dataset curation.

Additional research challenges arise when considering techniques that maintain the confidentiality of metadata in motion but permit metadata sharing between different analyses. An open research question is how access control on metadata can be implemented effectively using existing operating system and file system primitives, such as access control lists or capabilities. One challenge is that the granularity of control is commonly a file, yet large-scale scientific simulations commonly store hundreds of datasets in a single petabyte-sized file. A promising research avenue is devising fine-grained control mechanisms for metadata management for exascale scientific applications.

5 Related Work

The importance of metadata and provenance has been recognized in many different domains. In the Web domain, the Semantic Web is a collaborative standardization effort to formally represent knowledge. The Semantic Web community has created a number of standards and software tools, such as RDF [37], RIF [39], OWL [33], SPARQL [43], etc. to achieve this. Despite these efforts, the Semantic Web has not yet been universally embraced. Many efforts have proposed and developed for organizing scientific metadata into domain-specific vocabularies ("ontologies") allowing machines to understand and extract the semantic meaning of data [50]. These efforts, however, have been limited to specific application domains and standardization does not extend to generic scientific metadata.

Karma [25] is a stand-alone tool that collects and represents provenance information for digital scientific data. The Karma tool can collect file-based provenance information by automatically modifying batch job scripts [9], extract provenance information from log files [16], and visualize provenance [10]. Prior work has also suggested interfaces to access provenance information. Karvounarakis et al. [26] proposed ProQL, a querying language for searching the lineage of data. Mani et al. [30] proposed query language constructs and Holland et al. [22] developed an interface called PQL for querying provenance.

There have also been efforts to systematically manage metadata for specific scientific domains. In the atmospheric sciences domain, Pallickara et al. [34] have proposed the Atmospheric Data Discovery System (ADDS) to index and search observational datasets. In the environmental research domain, the "'Data Near Here" system allows scientists to reuse and exchange data without relying on "experts" to convey what the dataset structure is [29, 31].

Scientific metadata storage must be highly available and resilient to failures. Because metadata includes information on the physical location and layout of scientific data, it may be impossible to understand the data if the metadata is not accessible. Many scientific data management systems therefore store metadata in a relational DBMS for durability. SciDB [40] uses PostgreSQL for storing the shape and the location of each dataset fragment. The "Data Near Here" system also uses PostgreSQL for metadata storage [31]. ROARS, a data repository used by a biometrics research lab at the University of Notre Dame [6], stores metadata using MySQL. Not all metadata, however, can be universally represented using a fixed and structured relational schema. Hence, traditional relational database systems can sometimes be unnatural choices for storing metadata that cannot be efficiently represented using the relational data model. The SPOT suite [44] uses MongoDB for storing light-source data and simulations. The JGI Archive and Metadata Organizer (JAMO) [24] archives data related to gene sequences and also stores metadata in MongoDB.

Prior work has studied efficient techniques to store and query generic metadata information within a workflow. Shankar et al. propose techniques to integrate scientific workflow management in a relational database system [41]. Bowers and Ludäscher have set the theoretic foundations for propagating semantic annotations within [4]. Callahan et al. have proposed VisTrails, a workflow system that supports visual data exploration and visualization of provenance information [7]. Bao et al. have developed a dynamic labeling scheme that allows data items to be efficiently labeled with fine-grained provenance information [2]. Queries about whether two data items in different phases of a workflow are related can be expressed as reachability queries. Finally, Heinis and Alonso have proposed to represent provenance dependency graphs as intervals, and show how to query these intervals efficiently [21].

6 Conclusions

Ad hoc scientific data exploration and analysis today relies on a domain expert who can understand the structure of the data and the nuances of the process that generated it. Integrated metadata acquisition and management can significantly increase the reuse value of scientific datasets and the productivity of scientists. The efficiency of scientific exploration increases as data analysis tasks can be directed more judiciously using the insights stored and conveyed as metadata. This will accelerate exploratory analysis of scientific data, and increase the longevity and reuse of curated data and insights. Our vision for integrated and ubiquitous metadata management is a critical stepping stone towards achieving physical and logical data independence for extreme-scale scientific applications.

Acknowledgments

This work is supported in part by the Director, Office of Laboratory Policy and Infrastructure Management of the U.S. Department of Energy under contract DE-AC02-05CH11231, the U.S. National Science Foundation under grant IIS-1422977 and a Google Research Award.

References

[1] ADIOS: ADaptable I/O System. `https://www.olcf.ornl.gov/center-projects/adios/`.

[2] Z. Bao, S. B. Davidson, and T. Milo. Labeling workflow views with fine-grained dependencies. *PVLDB*, 5(11):1208–1219, 2012.

[3] The Blue Brain Project - EPFL. `http://bluebrain.epfl.ch/`.

[4] S. Bowers and B. Ludäscher. A calculus for propagating semantic annotations through scientific workflow queries. In *EDBT Workshops*, pages 712–723, 2006.

[5] BRAIN Initiative. `https://en.wikipedia.org/wiki/BRAIN_Initiative`.

[6] H. Bui. *A rich metadata filesystem for scientific data*. PhD thesis, University of Notre Dame, May 2012.

[7] S. P. Callahan, J. Freire, E. Santos, C. E. Scheidegger, C. T. Silva, and H. T. Vo. VisTrails: Visualization meets data management. In *Proceedings of the 2006 ACM SIGMOD*, SIGMOD '06, pages 745–747, 2006.

[8] M. Chaarawi and Q. Koziol. HDF5 Virtual Object Layer. Technical report, Available: https://confluence.hdfgroup.uiuc.edu/display/VOL/Virtual+Object+Layer, 2011.

[9] Y.-W. Cheah, S. R. Canon, B. Plale, and L. Ramakrishnan. Milieu: Lightweight and configurable big data provenance for science. In *BigData Congress*, pages 46–53, 2013.

[10] P. Chen, B. Plale, Y.-W. Cheah, D. Ghoshal, S. Jensen, and Y. Luo. Visualization of network data provenance. In *HiPC*, pages 1–9, 2012.

[11] Conventions for the standardization of NetCDF files. `http://tinyurl.com/pnfvbp8`.

[12] P. Cornillon, J. Gallagher, and T. Sgouros. OPeNDAP: Accessing data in a distributed, heterogeneous environment. *Data Science Journal*, 2:164–174, 2003.

[13] R. Dunlap, L. Mark, S. Rugaber, V. Balaji, J. Chastang, L. Cinquini, C. DeLuca, D. Middleton, and S. Murphy. Earth system curator: metadata infrastructure for climate modeling. *Earth Science Informatics*, 1(3-4):131–149, 2008.

[14] Earth system grid (ESG). `https://www.earthsystemgrid.org`.

[15] Earth system modeling framework (ESMF). `http://www.cisl.ucar.edu/research/2005/esmf.jsp`.

[16] D. Ghoshal and B. Plale. Provenance from log files: a BigData problem. In *EDBT/ICDT Workshops*, pages 290–297, 2013.

[17] GLEAN: In situ Visualization and Analysis. `http://tinyurl.com/l5lqa5z`.

[18] J. Gray, D. T. Liu, M. A. Nieto-Santisteban, A. S. Szalay, D. J. DeWitt, and G. Heber. Scientific data management in the coming decade. *SIGMOD Record*, 34(4):34–41, 2005.

[19] J. Gray and A. Reuter. *Transaction Processing: Concepts and Techniques.* Morgan Kaufmann Publishers Inc., San Francisco, CA, USA, 1st edition, 1992.

[20] A. Gupta, C. Condit, and X. Qian. BioDB, an ontology-enhanced information system for heterogeneous biological information. In *Journal of Data and Knowledge Engineering*, pages 1084–1102, 2011.

[21] T. Heinis and G. Alonso. Efficient lineage tracking for scientific workflows. In *SIGMOD Conference*, pages 1007–1018, 2008.

[22] D. A. Holland, U. Braun, D. Maclean, K.-K. Muniswamy-Reddy, and M. Seltzer. Choosing a data model and query language for provenance. In *IPAW*, 2008.

[23] IPCC fifth assessment cycle. `http://www.ipcc-wg2.gov/AR5-tools/`.

[24] The JGI Archive and Metadata Organizer (JAMO). `http://tinyurl.com/qypz2c2`.

[25] Karma provenance collection tool. `http://d2i.indiana.edu/provenance_karma`.

[26] G. Karvounarakis, Z. G. Ives, and V. Tannen. Querying data provenance. In *Proceedings of the 2010 ACM SIGMOD International Conference on Management of Data*, SIGMOD '10, pages 951–962, 2010.

[27] D. Korenblum, D. Rubin, S. Napel, C. Rodriguez, and C. Beaulieu. Managing biomedical image metadata for search and retrieval of similar images. In *Journal of Digit Imaging*, pages 739–748, 2011.

[28] P.-Å. Larson, S. Blanas, C. Diaconu, C. Freedman, J. M. Patel, and M. Zwilling. High-performance concurrency control mechanisms for main-memory databases. *PVLDB*, 5(4):298–309, 2011.

[29] D. Maier, V. M. Megler, A. M. Baptista, A. Jaramillo, C. Seaton, and P. J. Turner. Navigating oceans of data. In *SSDBM*, pages 1–19, 2012.

[30] M. Mani, M. Alawa, and A. Kalyanasundaram. Query language constructs for provenance. In *IDEAS '11*, pages 254–255, 2011.

[31] V. M. Megler and D. Maier. Finding haystacks with needles: Ranked search for data using geospatial and temporal characteristics. In *SSDBM*, pages 55–72, 2011.

[32] Numerical model metadata initiative. `http://climate.ncas.ac.uk/NMM/ipcc/index.php`.

[33] OWL web ontology language reference. `http://www.w3.org/TR/owl-ref/`.

[34] S. L. Pallickara, S. Pallickara, and M. Zupanski. Towards efficient data search and subsetting of large-scale atmospheric datasets. *Future Generation Comp. Syst.*, 28(1):112–118, 2012.

[35] NetCDF climate and forecast (CF) metadata convention. `http://cf-pcmdi.llnl.gov/`.

[36] Program for integrated earth system modelling (PRISM). `http://tinyurl.com/pp5lj65`.

[37] Resource description framework (RDF). `http://www.w3.org/RDF/`.

[38] R. Rew and G. Davis. NetCDF: an interface for scientific data access. *Computer Graphics and Applications, IEEE*, 10(4):76–82, July 1990.

[39] RIF overview. `http://www.w3.org/TR/rif-overview/`.

[40] SciDB: open source data management and analytics software for scientific research. `http://www.scidb.org`.

[41] S. Shankar, A. Kini, D. J. DeWitt, and J. F. Naughton. Integrating databases and workflow systems. *SIGMOD Record*, 34(3):5–11, 2005.

[42] E. Soroush and M. Balazinska. Time travel in a scientific array database. In *ICDE*, pages 98–109, 2013.

[43] SPARQL query language for RDF. `http://www.w3.org/TR/rdf-sparql-query/`.

[44] The SPOT Suite project. `http://spot.nersc.gov/`.

[45] The HDF Group. Hierarchical Data Format, version 5, 1997-NNNN. http://www.hdfgroup.org/HDF5/.

[46] K. Q. Tran, S. Blanas, and J. F. Naughton. On transactional memory, spinlocks, and database transactions. In *ADMS@VLDB*, pages 43–50, 2010.

[47] UK Data Archive - Research Data Lifecycle. `http://www.data-archive.ac.uk/create-manage/life-cycle`.

[48] R. V., W. Daughton, H. Karimabadi, and F. S. Mozer. Influence of the lower-hybrid drift instability on magnetic reconnection in asymmetric configurations. *Phys. Rev. Lett.*, 108:185001, 2012.

[49] X. Wang, R. C. Burns, and T. Malik. LifeRaft: Data-Driven, Batch Processing for the Exploration of Scientific Databases. In *CIDR*, 2009.

[50] N. Washington and S. Lewis. Ontologies: Scientific data sharing made easy. *Nature Education*, 1(3):5, 2008.

[51] G. Weikum and G. Vossen. *Transactional Information Systems: Theory, Algorithms, and the Practice of Concurrency Control and Recovery.* Morgan Kaufmann Publishers Inc., San Francisco, CA, USA, 2001.

[52] J. C. Wright, M. Greenwald, J. Stillerman, G. Abla, B. Chanthavong, S. Flanagan, D. Schissel, X. Lee, A. Romosan, and A. Shoshani. The MPO API: A tool for recording scientific workflows. In *Fusion Engineering and Design*, pages 754–757, 2014.