SCI\SPACE: A Scientific Collaboration Workspace for File Systems in Geo-Distributed HPC Data Centers

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Abstract—Future terabit networks are committed to dramatically improving big data motion between geographically dispersed HPC data centers. The scientific community takes advantage of the terabit networks such as DOE’s ESnet and accelerates the trend to build a small world of collaboration between geospatial HPC data centers. It improves information and resource sharing for joint simulation and analysis between accelerates the trend to build a small world of collaboration between geospatial HPC data centers. It improves information and resource sharing for joint simulation and analysis between the HPC data centers. In this paper, we propose to build SCI\SPACE (Scientific Collaboration Workspace) for collaborative data centers. It provides a global view of information shared from multiple geo-distributed HPC data centers under a single workspace. SCI\SPACE supports native data-access to gain high-performance when data read or write is required in native data center namespace. It is accomplished by integrating a metadata export protocol. To optimize scientific collaborations across HPC data centers, SCI\SPACE implements search and discovery service. To evaluate, we configured two geo-distributed small-scale HPC data centers connected via high-speed Infiniband network, equipped with LustreFS. We show the feasibility of SCI\SPACE using real scientific datasets and applications. The evaluation results show average 36% performance boost when the proposed native-data access is employed in collaborations.

I. INTRODUCTION

In recent years, we are experiencing a data explosion: almost 90% of today’s data has been produced in the last two years, with data being produced in the magnitude of petabytes\textsuperscript{1}. A weather company reported that more than 20 terabytes of data being generated each day for storing temperature readings, wind speeds, barometric pressures and satellite images across the globe\textsuperscript{2}. Several DOE’s HPC (High Performance Computing) leadership-computing facilities, such as OLCF (Oak Ridge Leadership Computing Facility), NERSC (National Energy Research Scientific Computing Center), and ALCF (Argonne Leadership Computing Facility), generate hundreds of petabytes of simulation data annually and are projected to generate in excess of one exabyte per year\textsuperscript{3}. To accommodate such growing volumes of data, science and research communities are deploying larger, well-provisioned geo-distributed storage and computation HPC clusters\textsuperscript{3}.

In the HPC data centers, data transfer nodes (DTNs) are supplied to access the provisioned storage and compute clusters\textsuperscript{4}. External access using DTN mitigates security risks. A top such DTNs, scientists and researchers across different HPC data centers collaborate by sharing simulation and analytical data for science research and discovery\textsuperscript{5},\textsuperscript{6}. Particularly, the high-speed terabit network connections between HPC data centers expedite such collaborations. DOE’s ESnet currently supports 100 Gb/s of data transfers between DOE facilities. In future deployments, it is expected to support 400 Gb/s followed by 1Tbps\textsuperscript{7}. Generally, scientists and their collaborators using the DOE facilities typically have access to additional storage and compute resources at multiple geo-distributed HPC data centers. By exploiting various computing resources at geo-dispersed HPC data centers, scientists efficiently perform simulations and data analyses, resulting in fast scientific discoveries. For instance, an OLCF petascale simulation needs nuclear interaction datasets processed at NERSC\textsuperscript{8}. Similarly, scientists in ALCF validate their simulation results by comparing them with climate observation datasets at ORNL data center\textsuperscript{8}. This collaboration between data centers is accompanied by data movement between OLCF and ALCF.

A traditional workflow of scientific collaborations is as follows: the scientists at different facilities engage remote access tools such as SSH to connect remote sites and find the required datasets, copy the datasets to local sites via data transfer tools such as bbcp and scp, and afterwards, execute the analysis\textsuperscript{8}. Figure\textsuperscript{1} depicts the traditional collaboration model between two collaborators from different HPC data centers. However, such an approach does not work when multiple HPC data centers are involved, because a SSH session is unable to present a single, unified workspace out of all shared datasets from multiple data centers. Therefore, it is crucial to render a unified view of shared datasets to all the collaborators via a collaborative namespace. Existing studies, such as CFS\textsuperscript{6}, OceanStore\textsuperscript{9}, Campaign Storage\textsuperscript{10}, and UnionFS\textsuperscript{11} can provide an aggregated storage space, but not the collaborative namespace. The collaborative namespace in SCI\SPACE eliminates the need for laborious data transfers and manage, which have been conducted manually by scientists, by allowing fine-grained sharing configurations for individual datasets.

Above all, scientists in collaboration might require analyzing the specific datasets based on certain conditions, for example, an analysis on a dataset which is generated from a satellite at a certain location for a specific period of time, e.g., from a start point to an end point. Existing parallel and distributed file systems do not directly support such advanced, data-aware search queries. A common approach to provide the advanced data search service is to build a metadata indexing layer, using an external database system, between the application and the file system. However, this not only requires modifications to both applications and the file system, but also forces scientists to use the SQL interface instead of the familiar file system interface. TagIT\textsuperscript{12} offers data extraction and discovery service on top of a file system namespace.
Bulk data transfer makes the following contributions: connected via the high-speed network. Specifically, this paper builds collaborations in a paradigm where HPC data centers are overlapping collaborations, which is not addressed by any of the existing studies. Therefore, it is essential to provide a collaboration workspace model to allow practical and powerful collaborations in a paradigm where HPC data centers are connected to high-speed networks.

To address the aforementioned challenges, we propose to build SCISPACE, a scientific collaboration workspace framework for file systems across geo-distributed HPC data centers connected via the high-speed network. Specifically, this paper makes the following contributions:

- SCI SPACE promotes the collaboration activities among the scientists at remote HPC sites for data sharing, joint simulation, and analysis. The proposed service framework provides a virtual abstraction on top of multiple dissimilar file systems and presents a global unified view of shared datasets to all the collaborators. SCI SPACE allows a native data access, e.g., local file write, which allows high performance file operations and minimizes modifications to the existing applications and file systems. Any changes to the local data center file system are transparently applied to the collaboration workspace by Metadata Export Utility (MEU).
- SCI SPACE offers efficient Scientific Discovery Service (SDS) integrated on top of the collaboration workspace to facilitate the scientific workflow. Specifically, SCI SPACE provides a multi-mode metadata extraction service based on application’s requirement. Additionally, to allow a single scientist to participate in multiple collaborations, SCI SPACE supports a template namespace. Using the template namespace, scientists can associate data sharing options, such as shared and private namespaces, to individual collaborations.
- We conduct a comprehensive evaluation of SCI SPACE by building a collaboration between two small-scale geo-distributed HPC data centers with Lustre file systems [13]. We compare the performance of our framework with UnionFS [11]. In addition to synthetic datasets, we also use real scientific datasets and applications. Our evaluation demonstrates that SCI SPACE outperforms the traditional approach by 36% on average, in real collaborations.

II. RELATED WORK

Figure 1 represents a scientific collaboration environment between two geo-distributed HPC data centers, i.e., ORNL and NERSC, allowing the remote collaborators to access the local facilities [8]. Existing storage systems, such as GFarm [14], XtremFS [15], iRODS [16], Hadoop [17], Lustre [13], and GlustreFS [19], can provide an aggregate view of data stored on multiple nodes within a single facility. However, such systems attain the aggregated storage view by deploying an identical storage interface on each storage node and do not support the unification of dissimilar file systems. Campaign Storage [10] and OceanStore [9] offer an aggregate storage interface and are designed to provide storage and data access facility to geo-distributed sites. However, in these systems, users cannot selectively publish datasets. More importantly, shared datasets always need to be stored via the aggregate storage interface, CFS [6] allows the read-only access to shared data whereas, read-only access is not aligned with collaboration activities. The file system unification studies, including WheelFS [20], UnionFS [11] and GBFS [21], are focused on providing a full-featured file system atop deployed file systems. However, they do not provide collaboration-oriented features, such as data sharing control and advanced data discovery services.

Another important factor of the scientific collaboration is tight coupling to POSIX interface. Traditionally, most scientific applications have been written to store and retrieve datasets using POSIX-compatible file systems [22]. Introducing a new interface for the purpose, e.g., relational databases [2], requires costly migration of existing datasets and unnecessary learning hassles to scientists. In addition, scalable and efficient scientific discovery and search services, e.g., extracting desired datasets from billions of file system entries, are becoming an important component in HPC. Recent studies, such as VSFS [22], Klimatic [5], and TagIt [12], integrated such data management services at the file system layer, instead of deploying additional database systems. Providing the data management services are also important in collaboration environments, because it can eliminate unnecessary data transfers between facilities by quickly identifying and extracting datasets of interest.

SCI SPACE provides a virtual collaboration workspace to facilitate scientific collaborations. The collaboration workspace provides common data visibility and also supports the advanced data discovery services in a high-speed network connectivity. It is crucial to present a single pathname to view and share a dataset, even when multiple data centers or sites participate in the collaboration. Moreover, the collaboration workspace should support advanced data discovery services, e.g., attribute-based file search queries, to effectively retrieve desired datasets and avoid unnecessary data transfers. In addition, it is common that a scientist participates in multiple collaborations [23]. To the best of our knowledge, none of existing systems directly support multiple collaborations, which we address via providing template namespace. SCI SPACE offers a gluing POSIX-compliant interface atop dissimilar file systems from different geo-distributed HPC data centers.

III. SCI SPACE: SCIENTIFIC COLLABORATION WORKSPACE

In this section, we present our key design goals and discuss the design and implementation of SCI SPACE in detail.

A. Goals

- Collaboration Workspace: The key design goal is to provide consolidated data visibility to all collaboration data.
centers under a single uniform namespace. A workspace is layered atop multiple dissimilar file systems mounted on data transfer nodes, and presents a common unified data view to all participants in the collaboration.

- **Native-Data Access Support**: To keep minimal modifications while achieving high performance, we consider it important to support for local writes and reads using local data center’s file system namespace.

- **Multi-Namespace and Selective Data-Sharing**: In real-world scenarios, it is common that a single scientist is involved in multiple collaborations. Moreover, offering the ability to selectively share data via different namespaces for each collaborator. Thus, we added privilege in our design to manage multiple collaboration workspaces.

- **Efficient Data Discovery and Search**: In geo-distributed collaborations, the extraction of required and useful data is of high significance. Additional performance overhead and network cost can be incurred if the required dataset is not intelligently retrieved. To incorporate such intelligence, we consider the scientific discovery and search service as an important design goal. **SCI SPACE** supports attribute-based data search facility.

### B. Scientific Collaboration Workspace

The proposed collaboration model renders a global picture of shared data to all the participants in the collaboration. An architectural overview of the proposed collaboration workspace is shown in Figure 2.

![Fig. 2: An Architectural Overview for SCI SPACE.](image)

**1) Unified Virtual File System Layer**: The Scientific Collaboration Workspace empowers SCI SPACE to elude the need for modifications to existing scientific applications and file system architecture. The intention to keep the existing application and storage architecture intact drives the need to implement a file system interface which can offer POSIX semantics. Besides, all collaboration participating geo-dispersed data centers grants access to shared resources such as storage and compute nodes via single or multiple DTNs. The effective utilization of provided multiple DTNs is also an essential viewpoint which needs to be considered. If not properly approached, it can lead to bottlenecks, i.e., multiple collaborators accessing a single DTN. To this end, our Scientific Collaboration Workspace is equipped with a POSIX-like file system API and provides all the basic file system operations. To manage the metadata effectively, we employ a distributed metadata architecture and details are presented in next subsection III-B2.

**2) Metadata Management**: Metadata is of high significance in file systems because it is the key input to all file system services. In collaboration environments, the need to minimize the metadata bottleneck originates when collaborator traffic increases. We adopted distributed metadata to reduce metadata bottlenecks caused by the central metadata management approach. Distributed metadata provides more efficient scientific search and indexing services than a centralized indexing approach.

The metadata service in **SCI SPACE** is running on every DTN from all participating data centers. The reason to execute metadata services on DTNs is manifold, (i) we can effectively utilize the DTNs, (ii) storing metadata globally enables us to...
provide metadata to all the collaborators mounting SciScape, and (iii) we can exploit multiple available DTNs as distributed metadata services for efficient scientific discovery and indexing as compared to centralized metadata approach. To keep our design scalable, we split metadata into multiple partitions. This partitioning helps in obtaining a fair load-distribution across available DTNs. Each instance of metadata partition acts as a DB-Shard (database shard).

Specifically, each DTN maintains two DB shards, i.e., metadata service shard and discovery service shard, as shown in Figure 4. We maintain two different types of metadata, i.e., file system metadata and indexing metadata. The file system metadata, such as filename, size, owner, and the path, is synchronously updated when a write request is received. The indexing metadata includes metadata of scientific dataset headers (such as HDF5 and NetCDF self-contained attributes) and user-defined indexing attributes. For index metadata, we provide both synchronous and asynchronous DB update mechanisms. In synchronous DB update, the file indexing and metadata extraction is performed when a write request is received. It incurs high overhead but it can be masked under FUSE layer overhead. Whereas, in asynchronous DB update, the file indexing and metadata extraction is conducted later after file is stored. Only a single message is sent to indexing service to register the file for indexing and metadata extraction. When to conduct the indexing and metadata extraction depends on pre-defined threshold such as time, size and file count. The asynchronous DB update exhibits inconsistency between the file system metadata and the indexing metadata, depending on how early the metadata extraction and indexing is performed after the corresponding file operation. We further explain the pros and cons of two DB update mechanisms in Section III-B3.

This distributed metadata architecture is tightly coupled within the collaboration workspace. We adopt an index data structure to promote effective lookup and search queries on top of relational database to enable file attribute based retrieval. We do not use key-value stores, as our metadata indexing approach requires multiple associations, e.g., linking a single file with multiple attributes or single attribute to multiple files. The schema for collaboration and indexing metadata is shown in Figure 4. Note that such attribute-based file retrieval is not possible in the traditional approach without performing a costly exhaustive search.

SciScape obtains two significant benefits by integrating file indexing and attribute extraction at file system layer: (i) effective execution of metadata-intensive I/O operations such as file name and path mappings on specific data center, (ii) no crawling/file lookup required on multiple file system namespaces, (iii) empowering search and query based on custom-defined attributes, file system stat attributes and scientific dataset attributes (such as HDF5 self-contained attributes).

3) Local-Writes and Export Protocol: The file system interface of SciScape (scifs) allows collaborators to seamlessly access local and remote datasets in the collaboration workspace. However, the additional file system layer, written using the FUSE framework in our prototype (Section III-B1), may degrade the overall I/O performance. To avoid such performance degradation, SciScape supports local-writes, i.e., writing data directly to the local data center file system instead of the collaboration workspace (FUSE layer). Through the local-writes, SciScape can deliver the native performance of the local data center file systems when collaborators can exploit the local file systems. Furthermore, the local-writes also reduce the network traffic across the sites and simplify the consistency and resilience managements due to direct storage at local data center namespace. However, datasets that have been written through the local-writes are not directly visible inside the collaboration workspace, and thus should be properly propagated to the file system namespace of the collaboration workspace.

To assist local-writes, SciScape features Metadata Export Utility (MEU), which commits all unsynchronized metadata of locally-written datasets to the file system namespace of the collaboration workspace. In addition, collaborators can explicitly trigger such commits. This concept works in a similar fashion to git local and remote repository management. In our design, because datasets written via the local-write are stored in permanent storage (local data-center file system) only their metadata needs to be synchronized with the collaboration workspace namespace. MEU appropriately synchronizes such metadata into the collaboration workspace namespace. In addition, MEU allows a fine-grained control for sharing the datasets, e.g., when a collaborator wants to share only subset of a dataset via collaboration workspace.

The local-write and MEU workflow is shown in Figure 5. MEU scans the files and directories recursively from a certain local directory, such as /home/project. During the scan, it checks the extended attribute sync of each file and directory in a pathname. For example, to examine /foo/bar/hello.hdf5, MEU first checks the extended attribute of foo. If the flag is true, MEU skips the entire directory because all files and directories under foo have already been synchronized. Otherwise, MEU enters the directory and scans entries. Whenever any change occurs inside a directory, we modify the flag of the parent directory of the file or directory (in the example, bar is the parent of hello.hdf5). Once the scan phase finishes, we add an extended attribute to all unsynchronized files. When MEU synchronizes the metadata, it packs all unsynchronized metadata into a single message to minimize the synchronization overhead.

4) Template Namespace: SciScape is intended to effectively satisfy the needs for various types of collaborations. For instance, a collaborator may require a dedicated workspace for own research, simulation, and analytical jobs. Also, a collaborator may be involved in multiple collaborations simultaneously. Cloud data storage systems such as Dropbox and
Google Drive permits sharing data with multiple users, and a user can participate in multiple projects and collaborations. Based on these practical use-cases, SciSpace provides a namespace management module, Template Namespace, based on the distributed metadata management architecture. Collaborators can define multiple namespaces in SciSpace with the scope of each namespace (local/global). Figure 4 shows the association between Template Namespace and other metadata in SciSpace. In specific, when a file is written, its pathname determines the namespace, which in turns defines the scope of the file content. If a namespace scope of a file is local, the file is only visible to the owner of the file. Similarly, if the scope is global, the file becomes visible to any collaborators within the collaboration workspace, e.g., a remote collaborator.

5) Scientific Discovery Service: Extracting a desired dataset from billions of data files remains a central interest of the science and research communities. Particularly, a support of Scientific Discovery Service (SDS) within the collaboration workspace provides the following benefits; i) it frees collaborators from retrieving undesired data to local data centers via data transfer tools such as bcp [24], LADS [8], and ii) it circumvents manual dataset screening phase in scientific workflows performed before analysis. However, since the SDS service entails additional processing for generating per file indexes, it may incur a certain performance overhead. Therefore, if such an indexing is not required on a certain dataset, it is favorable to skip the indexing for the dataset to avoid the overhead. For instance, an application may only require a storage space without having any subsequent analysis tasks. In addition, it is possible that a scientist does not need such an indexing feature for a certain dataset. To support such various requirements, SciSpace provides three different metadata extraction modes.

- **Inline-Sync**: In this mode, write operation includes both data storage and metadata extraction in a synchronous way. As depicted in Figure 6, a write operation completes only after all the metadata is extracted and indexed. This mode aims to facilitate applications that require both storage space and immediate analysis on produced datasets. Although the Inline-Sync mode provides a strict consistency between datasets and the index database, its synchronous metadata can significantly slow down the individual I/O operations.

- **Inline-Async**: To reduce the increased I/O wait time, we propose Inline-Async mode, that injects partial de-coupling between storage and extraction operation. As shown in Figure 6, the total file write time in Inline-Async does not include the metadata extraction process. In specific, we adopt a queue-based metadata extraction architecture, where an indexing request message is enqueued when a file is written. SDS asynchronously dequeues messages and index data accordingly. This mode specifically targets environments with offline or delayed analysis after data generation. It includes FUSE and negligible message enqueue overhead.

- **LW-Offline**: To support indexing on top of local-writes (LW), we require offline indexing mode which directly performs the metadata extraction within the data center file system namespace. This mode aims to facilitate cases when datasets are stored via the local namespace and high-performance is expected. The indexing service is triggered on the DTN directly. The write operation includes no FUSE overhead due to native access.

In the scientific community, the HDF5 and NetCDF datasets are most commonly used data formats [25]. SDS utilizes the HDF5 library [25] to extract all the attributes from the HDF5 file. Collaborators can specify attributes to index data in SciSpace. The SDS validates the data for matching attributes defined by the collaborator. If the match is found, the entry (attribute, file, value) is recorded in the Discovery shard as shown in Figure 4. In addition, we also offer manual or collaborator-defined tagging, where a collaborator is facilitated to tag file or group of files with custom attributes. The simple attribute structure consists of attribute.name which refers to attribute name, attribute.type refers to attribute datatypes, and attribute.value refers to the value of an attribute. In the scope of current work, we provide only three types of attribute types, i.e., integer numbers, floating point numbers, and texts. We plan to extend our implementation to include range-based attribute datatypes.

SciSpace provides a query interface via a command line utility. Using query interface, collaborators can easily query the desired contents/files within the collaboration workspace. The command line utility supports operators inside a query string, such as equal (=), greater (>), and less (<). For the text datatype, we provide equal (=) and like (like) operation.

SciSpace currently delegates the fault-tolerance, replication, and data consistency managements to distributed and parallel file systems inside data centers. In fact, SciSpace inherits all these features from data center equipped file systems, because it merely adds a thin virtual abstraction layer on top of the mountpoints of such file systems. However, we consider the collaboration workspace metadata replication as an important factor and plan to support the metadata replication in future.
TABLE I: Description of Evaluation Test-bed Setup.

| Component | Description |
|-----------|-------------|
| Collaboration | 2 Data Centers |
| Storage | Lustre PFS for each Data center |
| Lustre | 4 Nodes (2 x MDS, 2 x OSS) |
| MDS | 24 Intel Xeon E5-2650 CPU Cores, RAM 128 GB, 1 x 6.3 TB MDT |
| OSS | 16 Intel Xeon E5-2650 CPU Cores, RAM 64 GB, 11 x 7.2 TB RAID-0 OSTs |
| DTNs | 24 x Intel Xeon E5-2650 @2.20GHz |
| Collaborators | 1-24 Collaborators |
| CPU Cores | 24 x Intel Xeon E5-2650 @2.20GHz |
| Memory | 128 GB |
| Network | Infiniband EDR (100Gbps) |
| OS | CentOS Release 7.3 Kernel v3.10 |

IV. EVALUATION

A. Implementation

We implemented SCISPACE using the FUSE’s high-level API v2.9.4 [26]. Our implementation fully complies with POSIX standards and shows UNIX-like semantics and directory structure. A generic messaging protocol is employed to interact with all the components of SCIPLACE, accomplished via Google Protocol Buffers. Specifically, metadata service and scientific discovery service running on each DTN are implemented based on the client-server model using gRPC. The gRPC client can connect and interact with the metadata server. In our implementation, the metadata client is integrated in collaboration workspace. SQLite is used as backend storage for each database shard. SCIPLACE source code consists of more than 3000 lines.

B. Experimental Setup

1) Testbed: We build a testbed for scientific collaboration on top of two geo-distributed data centers equipped with Lustre [13] connected via high-speed Infiniband EDR (100Gbps) network. Table I shows detail description of the testbed setup. We use 2 DTNs for each data center as Lustre clients and mount the DTNs via Linux NFS v4.0 on to the collaborator machine as shown in Figure 3. Note our target environment is that, data centers in collaboration are connected via a high-speed network such as ESNet’s 1Tbps network [7]. We believe our testbed configuration fairly emulates this situation. Particularly, in such a Terabit network environment, the network bandwidth between the data centers is higher than the PFS bandwidth of each data center. To accurately emulate this situation, we have configured the Lustre bandwidth of our testbed to be smaller than the IB EDR bandwidth, as in [3].

We compare the proposed SCIPLACE against a simple unification file system approach such as UnionFS [11], designed to merge several directories and file system branches. We implemented the prototype idea of UnionFS using FUSE for comparison with SCIPLACE and SCIPLACE-LW. In experiments, SCIPLACE refers to the use of collaboration workspace to read and write whereas, SCIPLACE-LW refers to use of the local file system namespace and can benefit with native-access support. In the rest of the paper, we refer the approach of the UnionFS as the baseline. All the experimental results show the average of multiple runs. We drop cache after each iteration of experiment from NFS mount points, DTNs, and Lustre OSSs to have authentic performance values.

Fig. 7: Performance analysis of SCIPLACE by varying Block-Size.

(b) Read

Fig. 8: Performance analysis of SCIPLACE varying Collaborators.

2) Workload: To evaluate the SCIPLACE performance, we used IOR [27] benchmark. We use 375 GB of synthetic dataset using IOR. The reason to use big dataset is to wipeout the caching effect. For real collaboration activities, we use scientific HDF5 datasets comprised of the ocean surface data measured at different time period across geodistributed locations by different scientific instruments. We downloaded the dataset of size 116 GB (4600 files) from MODIS-Aqua [28]. MODIS plays a vital role to predict global changes accurately enough to assist policymakers in making decisions concerning the protection of our climate [28]. We use two HDF5 applications, i.e., H5Diff and H5Dump in order to emulate real collaboration activities.

C. Scientific Collaboration Workspace

To evaluate the performance overhead of SCIPLACE framework, we run two sets of experiments (read, write) and compare baseline with two variants of the proposed framework, i.e., SCIPLACE and SCIPLACE-LW. (quoted as native-access).

In Figure 7(a)(b), we investigate the impact of block size in both write and read operations with a single collaborator. We observe that when the block size is less than 16KB, the write and read performance degrades in both baseline and SCIPLACE as compared to SCIPLACE-LW. The reason for the decrease in read and write operations is due to small-size transfer requests, FUSE layer overhead, and metadata contact points. Whereas, SCIPLACE-LW shows higher performance due to local-writes support and low metadata contact points. However, as we increase the block size, the write and read performance increases in all three approaches. In Figure 7(a)(b), the maximum throughput achieved by the baseline and SCIPLACE is same at a block-size of 512KB however, the SCIPLACE-LW shows higher performance in all test cases, in particular ranging from small block-size 4KB up to 512KB. The performance improvement window lies in range from 2% up to 70% when moving from big block-size to smaller block-size. The average performance improvement of all write test-cases is 16%. However, for read test-case, SCIPLACE-LW shows a consistent performance improvement in all test cases with an average of
41%. The performance degrades in baseline and SCISPACE due to several factors, first additional metadata querying for stat, second FUSE invokes five operations serially, getattr, lookup, create, write and flush and third, user and kernel space context switching overhead cannot be ignored. Whereas, in SCISPACE-LW case, we allow collaborators to write to local file system namespace and push the unsynchronized metadata to SCISPACE. We have no additional metadata querying and no FUSE overhead in SCISPACE-LW.

Next, we perform the experiment to show scalability of SCISPACE collaboration workspace by increasing number of collaborators. Figure 8 (a)(b) shows the impact of multiple collaborators in both read and write operation of all three approaches, i.e., baseline, SCISPACE and SCISPACE-LW. We use the same dataset of size 375GB via IOR and fix the block-size to 512KB to benefit the baseline and SCISPACE approach as compared to SCISPACE-LW. The results stand different from our observations in the previous experiment Figure7. As we vary the number of collaborators, the baseline, SCISPACE, and SCISPACE-LW show a consistent performance improvement. The reason for this improvement is manifold. First, baseline and SCISPACE get the benefit of NFS caching at server and Lustre OSS cache and parallelism. Second, due to effective and load-balanced utilization of available DTNs, i.e., in the baseline, we allocate each DTN equal priority and in SCISPACE, we configure round-robin request placement policy. However, SCISPACE-LW, we divide the number of collaborators on each DTN. Whereas, our SCISPACE-LW cannot benefit with NFS caching because it directly runs on local data center namespace and can only utilize the parallelism of deployed Lustre at the data center. The maximum performance boost when 24 collaborators are active in collaboration is; for write test-case, 16% and read test-case shows 28% boost when compared to baseline and SCISPACE. However, we consider it is important to show the reason for read performance degradation when collaborators number varies from 8-16. The reason behind is NFS caching. So, in baseline and SCISPACE when the cache is full, the flush operation is invoked and all the write I/Os get slow due to multi-level cache (NFS cache, Lustre OSS) flush operation in progress. On the contrary, SCISPACE-LW requires only single cache flush (Lustre OSS).

D. Metadata Export Utility

Metadata Export Utility (MEU) performance relies on the number of files, irrespective of file size. Our realistic dataset contains 4600 files (116 GB), which we believe is not sufficient to clearly show the performance of MEU. To show the effectiveness of the proposed approach using a single collaborator, we define a simple workflow. We create a zero-size file (count 5K-1M) via baseline, SCISPACE-LW and execute the MEU on top of SCISPACE-LW (Figure 9 (a)) to synchronize the metadata of files such as filename and location (File Mapping Schema in Figure 4). The baseline approach uses the common FUSE-based collaboration workspace. In SCISPACE-LW, all the files are created via local file system namespace however, it does not include the MEU export overhead. Whereas, SCISPACE-LW+MEU) includes the use of local file system namespace and MEU export overhead as well. The experimental results are shown in Figure 9(a). We observe that baseline creates a huge overhead which comes from increased contact points between collaboration workspace and metadata service. Each of the file system calls (such as attr, access, create, open) requires assistance from metadata service. Whereas, SCISPACE-LW requires no such additional metadata assistance. However, MEU recursively iterates the directories and create the a list of unsynced files and send message to metadata service on DTN. The SCISPACE-LW and SCISPACE-(LW+MEU)show a linear performance pattern. In MEU, we batch all the requests and send single RPC call to metadata service to minimize the message packing overhead.

E. Scientific Discovery Service

In this section, we show the performance of multiple metadata extraction modes. For this experiment, we use the 4 collaborators and real scientific HDF5 datasets (116 GB). We extract all the attributes (Search Attribute in Table II, from HDF5 files along with file system metadata (pathname, size, time, inode number etc.). We specifically present Inline-Sync, Inline-Async, and LW-Offline. We described each mode in detail in Section III.B3. The Inline-Sync and Inline-Async use SCISPACE collaboration workspace, whereas LW-Offline uses the local data center namespace. It indexes the files and update SDS shard accordingly.

Figure 9(b) shows the time breakdown analysis of all the data discovery modes. As expected, the Inline-Async and LW-Offline perform better with an improvement factor of 12% and 36% with 5 attributes when compared to Inline-Sync. Whereas, when 20 attributes are used, the performance boosted up to 56% in Inline-Async and 62% LW-Offline. The high time taken by Inline-Sync is mainly derived from I/O blocking. A single write I/O waits until all the indexing operations are complete. The indexing operations include opening HDF5 file, extracting metadata attributes, and recording the attributes in the database. Also, when we compare Inline-Async and LW-Offline, the performance in earlier one is 56% and later one is 62% as compared to Inline-Sync when 20 attributes are used. The reason for negligible performance overhead in Inline-Async as compared to LW-Offline is the result of additional gRPC calls and protobuf messages for enqueuing the index messages. However, LW-Offline operates directly on the local file system namespace and incurs no added messaging overhead.

Next, we discuss the search query latency. We measure the search query latency using 4 collaborators, each produces four types of 1000 queries. We select each query based on the defined attributes in the real HDF5 dataset, i) search the files generated at a certain location, ii) search the files with the particular instrument, iii) search the files including specific date, iv) search the files generated in day or night. We populate the SDS shards with indexes and show latency by varying hit-ratio. The hit-ratio is defined as the number of matching tuples in SDS shard over the total number of tuples in shard. The average latency of each query is listed in Table II. We have seen that when hit-ratio is less, i.e., the number of matching entries are only 25% of total entries, the query latency is very short up to 8-9 seconds. However, when we vary the hit-ratio to 100%, the high latency is experienced in all search queries. This increase in query latency is the result of message packing
and unpacking at SDS. The SDS translates the request message into SQL query and finds the required attributes in SDS shard, then query results are packed in a message and sent over the network. When the number of records returned in the SQL query is high, then latency increases. This internal message packing overhead leads us to show the hit-ratio comparison.

F. End-to-End Analysis for Scientific Collaborations

We conduct the experiments to compare end-to-end analysis times between baseline approach and SCISPACE with real HDF5 tools such as H5Diff (computing the difference between two HDF5 files) and H5Dump (converting HDF5 file to ASCII file). In the baseline approach, it first finds the datasets on different datacenters, then migrates the datasets from all locations to local data center and run applications. In particular, the search time increases as the number of files searched increases because it only allows file-name based search. On the other hand, collaboration namespace gives benefit in terms of first two steps; first, query time is constant irrespective of data size and file count. Second, no-migration is required because application can run directly on searched dataset without transferring datasets to the local data center. Figure 9(c) shows the result of H5Diff application. SCISPACE shows lower end-to-end run times than baseline for all cases of different files. We observe the same performance trend for the H5Dump application, however due to page limit, we do not show the H5Dump results.

V. CONCLUSION

In this work, we propose SCISPACE, a Scientific Collaboration Workspace which offers a virtually unified common workspace to collaborators in multi-data center collaborations. SCISPACE supports native-data access to achieve high-performance via metadata export protocol. Scientific discovery service reduces the scientific workflows by efficiently extracting the desired datasets via offering search query-like utility. We evaluated SCISPACE on top of two small-scale geo-distributed HPC data centers connected via Infiniband and equipped with Lustre. The evaluation confirms the usefulness of the SCISPACE.

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**TABLE II:** Search query latency (in seconds) by varying Hit-Ratio.

| Search Attribute | Hit-Ratio |
|------------------|------------|
|                  | 0% | 25% | 50% | 75% | 100% |
| Location (Text)  | 3.6| 9.7 | 14.6| 19.5| 24.5 |
| Instrument (Text)| 3.8| 9.5 | 14.7| 19.7| 24.6 |
| Date (Text)      | 3.9| 9.6 | 14.8| 19.7| 24.6 |
| Day or Night (Int)|3.2|8.9 |14.1|18.9|23.9 |

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