Apache Airavata Sharing Service

A Tool for Enabling User Collaboration in Science Gateways

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ABSTRACT

Science Gateways provide user environments and a set of supporting services that help researchers make effective and enhanced use of a diverse set of computing, storage, and related resources. Gateways provide the services and tools users require to enable their scientific exploration, which includes tasks such as running computer simulations or performing data analysis. Historically gateways have been constructed to support the workflow of individual users, but collaboration between users has become an increasingly important part of the discovery process. This trend has created a driving need for gateways to support data sharing between users. For example, a chemistry research group may want to run simulations collaboratively, analyze experimental data or tune parameter studies based on simulation output generated by peers, whether as a default capability, or through explicit creation of sharing privileges. As another example, students in a classroom setting may be required to share their simulation output or data analysis results with the instructor. However most existing gateways (including the popularly used XSEDE gateways SEAGrid, Ultrascan, CIPRES, and NSG), do not support direct data sharing, so users have

to handle these collaborations outside the gateway environment. Given the importance of collaboration in current scientific practice, user collaboration should be a prime consideration in building science gateways. In this work, we present design considerations and implementation of a generic model that can be used to describe and handle a diverse set of user collaboration use cases that arise in gateways, based on general requirements gathered from the SEAGrid, CIPRES, and NSG gateways. We then describe the integration of this sharing service into these gateways. Though the model and the system were tested and used in the context of Science Gateways, the concepts are universally applicable to any domain, and the service can support data sharing in a wide variety of use cases.

CCS CONCEPTS

• General and reference \rightarrow Design; • Human-centered computing \rightarrow Collaborative content creation; • Information systems \rightarrow Computing platforms; • Software and its engineering \rightarrow Open source model;

KEYWORDS

Apache Airavata, SciGaP, CIPRES, NSG, SEAGrid, Collaboration, Science Gateways, Groups, Sharing

1 INTRODUCTION

Science gateways are science-centric user environments and supporting cyberinfrastructure that enable broader and more effective use of scientific computing resources, applications, and data [6]. Because gateways allow users to perform operations on high end resources, authentication and authorization have long been cornerstones of gateway infrastructure [9],[17]. Authenticated access also supports another hallmark

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Use Case 1	Sharing and Revoking capabilities.
Use Case 2	Check Permission of a given Entity.
Use Case 3	Browse and Search within all accessible en-
	tities for a given user.

Table 1: Gateway Use cases for Collaboration

of gateways: the collection of user interactions into computational experiments that the researcher can use to monitor long running executions, retrieve results, and recall how specific results were achieved [7], [12], [13], [15].

Sharing results with colleagues and making certain results publicly available is the outcome of research. This is an example of user-driven authorization of something the user owns (data and metadata) rather than service provider-driven authorization of something the service provider owns (computing resources, licensed applications, etc). Despite the fundamental nature of sharing in research, this is not a first class capability within many popular gateways. This paper examines the requirements and provides an implementation for user-directed sharing, which we apply to several popular science gateways.

Our conceptual approach is based on group membership. Computational experiments are grouped (or tagged) into one or more organizational structures. In Apache Airavata, for example, "projects" contain experiments. These entities are by default privately owned by the creator. The extensions are obvious: give other users and groups of users privileges to read the contents of specific experiments and groups of experiments. A subset group of these users may have additional privileges to copy, modify and execute experiments and groups of experiments. For even these simple cases, however, we know from common examples such as UNIX groups that we must reason carefully about how to implement inherited permissions, the nature of ownership and its transfer, and similar issues.

2 ENABLING COLLABORATIONS WITHIN SCIENCE GATEWAYS USING GROUPS

Groups are a natural choice to implement the gateway collaboration requirements outlined above. Groups themselves are just collections of entities. Entities can be users, data collections (files, folders), resources (application software, hardware resources, quality of service), experiments. Figure 1 provides a high level architectural overview to plug in group management and sharing services to SEAGrid [12], CIPRES [7] and NSG science gateways [15]. Section 6 summarizes the collaboration requirements provided by Neuroscience Gateway User Community. We summarize the sharing usecases from these gateways into 4 broad categories (Table 1).

Generic implementations of groups, and "groups as a service" software exist as standalone tools and services and are integrated with common identity management software. LDAP Groups [16] and Grouper [1] are well known examples. Grouper is a comprehensive group management software and

can be deployed at university scale to manage complicated collections of users and other entities. Grouper can very well be adapted to meet the gateway Use Cases 1 and 2. But despite their power and flexibility in handling groups, the lack of flexible querying makes it not a good match for gateway Use Case 3.

The core of the gateway use cases is to enable "Browsing and searching" within accessible data. As users perform large number of computations, the sharable entities for a given user grows large. An implied requirement for retrieving shared results is to paginate the resultant entities. We could potentially use Grouper like software for sharing needs, but implementing the browse and search of artifacts will deviate the systems for their intended usage. More over the Grouper like solutions are designed to run at University scale and assume dedicated personal resources to setup and operate. Gateways require a much lighter weight solutions.

One other non-technical but pragmatic reason include governance of the project itself. There are certainly other open source alternative group management software. The distinction being a "open source" and being community managed via a governance model are summarized in [11]. Our hypothesis is that science gateway community require a light weight, gateway use case focused and open governed open source project to build key collaboration capabilities.

To address the limitations of existing generic group management software and to have the flexibility to implement the above gateway collaboration use cases, we propose a relational data model in which the relationship between groups, permissions and resources is explicitly named and directed. At the simplest conceptual level, this approach provides an unambiguous representation of permissions on access to users' projects and computational experiments. This is an important design consideration given the security implications of sharing results. It furthermore leads to a more efficient, if specialized, implementation of queries.

3 PROPOSED SOLUTION

We identify the concept of Sharing as the cornerstone in developing a user collaboration system. Sharing is a ternary relationship between three abstract concepts: "Actor", "Artifact" and "Permission" (see Figure 3). Our model is similar to other resource level security models available in cooperative models [14]. An actor can be a single user, a group of users or even a group of other groups. The concept of Artifact represents any data entities in a gateway (such as a project, an experiment or an output file) and the Permission captures the level of access that each actor has on the artifact associated in the sharing relationship. Sample sharing rule defined using this model can be expressed as User1 has READ permission to Experiment 1. In our model, we assume all sharing rules are explicitly defined; i.e no default behavior. To keep the model simple, we also do not support sharing rules defined as negations, such as DISALLOW (User1 has READ permission to Experiment 1). When an Artifact is created, by default the owner of the Artifact will be assigned with the

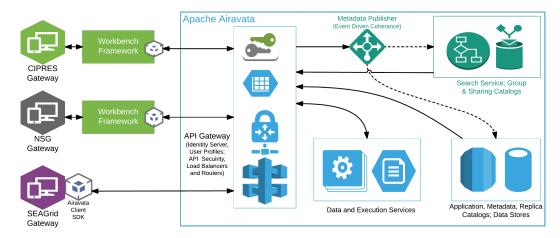


Figure 1: High level architectural overview. SEAGrid Gateway is built over Apache Airavata for all data and execution capabilities; CIPRES and NSG Gateways are built over Workbench Framework and are exploring use of Apache Airavata for Data Sharing capabilities. The paper focuses on Sharing Service (green color box) and existing literature on Airavata discuss other capabilities (blue colored boxes).

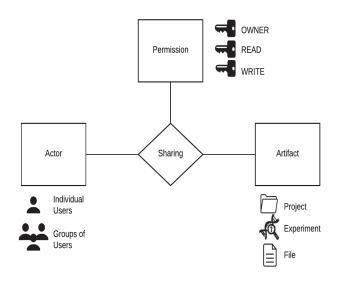


Figure 2: Relationship between the Actor, Permission, Artifact and Sharing concepts.

OWNER permission. This grants the global level permission on that particular Artifact. Next we look into each of these concepts in more detail.

Actor: An Actor can either be a single user or a group of users. A group will be owned by the creator of the group and can have other users or groups as child members. Child groups can in turn have other groups, which are owned by the same owner, as child members. The implementation avoids the creation of cyclic group memberships. A particular user can be a member of a group via direct membership or via indirect membership; i.e., by being a member of another nested

group or both. Based on the use cases, the direct and indirect membership can be enforced in different ways or need not be distinguished. When representing an actor we select a common metadata model that can represent individual user information as well as group information such that it can cater the usage requirements of the gateways.

Artifact: An artifact can be an arbitrary entity. A typical gateways describe artifacts to be a user project, job or a input/output file. In a more generic sense, an artifact can be any item that needs to be shared or have its access controlled. Artifacts can have hierarchical structures (i.e parent-child relationships). This hierarchy enables sharing at different granularities. For example, a user may want to share a project and all the nested child experiments and input/output files implicitly, or share only the project content (i.e project level metadata) without child entities. We do not allow Artifacts to have cyclic dependencies in their parent-child hierarchies. Similar to Actors, when representing Artifacts, we select a common metadata model, which includes fields such as name, description, created time, updated time, full text field and a placeholder for a binary object which can contain all other data.

Permission: Permission defines access types that an Actor can have on an Artifact in a sharing relationship. For example, User1 may have READ permission on Experiment1, which will only grant access to view things in Experiment1. Group1 may have WRITE permission on Experiment1 which would allow a Group1 member to write/update the content in Experiment1. Sometimes it is possible that one permission may subsume the access rights defined by another permission. For instance the OWNER permission (granted to the owner of an artifact) subsumes the access rights enforced by READ and WRITE permissions, thus defined as a super permission of both READ and WRITE permissions. A particular user may have READ permission either because the

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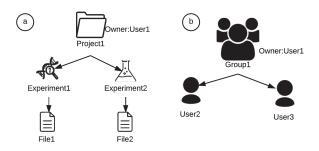


Figure 3: Hypothetical user collaboration scenario. (a) Artifact hierarchy owned by User1 and (b) Group hierarchy created by User1.

item is explicitly shared with READ permission or the user has another permission (e.g. OWNER) which subsumes the access rights of the READ permission. These kinds of relationships are captured in the form of a permission hierarchy. Similar to Actors and Artifacts these hierarchies also cannot have cyclic parent-child dependencies.

4 IMPLEMENTATION

To realize the science gateway use cases summarized in Table 1, we implemented the architecture discussed above. The relationships between entities guided us to select a relational database engine. The choice of the Object-Relational Mapping enables the underlying databases such as Derby and MySQL to be plugged in seamlessly to Apache Airavata. To simplify the implementation, individual Users are treated a special type of Group with a restriction to have one member.

Sample Scenario: We describe the sharing implementation using a hypothetical sample scenario. Let's say three users would like to define three permission types (OWNER, READ and WRITE), and collaborate on artifact types (PROJECT, EXPERIMENT, and FILE). User1 owns one project (Project1) in which contain two experiments (Experiment 1 and 2) each with a file (File 1 and 2). User1 creates a group (Group 1) two child members (User 2 and 3). We will now walk through all 4 gateway use cases for this scenario.

Sharing and Revoking: Initially only User1 has access to Project1 and all other nested artifacts (through the default assignment of the OWNER permission). If User1 wants to give READ permission to Project1 for User2, the lucid design facilities gateways to accomplish it in multiple ways. The most basic approach would be to explicitly share Project1 with User2 with READ permission. This operation corresponds to creating an entry in Sharing table which can be represented as:

```
INSERT INTO SHARING(ACTOR, ARTIFACT, PERMISSION) VALUES(
    User2, Project1, READ)
```

However this will allow User2 to READ Project1 and not any of its nested artifacts. If User2 also needs to have READ permission to all nested artifacts of Project1 we need to define sharing rules for all the nested artifacts rooted at Project1, either explicitly or implicitly. The implicit way to handle this is to add an additional field in the Sharing rule to capture this information. The explicit way to handle this is to traverse through the Artifact subtree and create sharing records for each nested Artifact. The two approaches can be represented as follows:

```
INSERT INTO SHARING(ACTOR, ARTIFACT, PERMISSION, CASCADE)
    VALUES(User2,Project1, READ, True)
```

There are tradeoffs in choosing between these two approaches. The implicit approach has constant time complexity at sharing time but requires complex and computationally expensive retrieval operations at inference time (i.e Check permission and Search operations). On the other hand, the explicit approach has O(n) time complexity (n is the number of artifacts in the subtree) and requires constant time complexity at inference time (assuming constant time retrieval using a database index). In a practical setting, most operations the sharing model should support will be inference type operations. Hence in our model we have decided to use the explicit approach.

To explain the need for CASCADE field, consider the following case. Assume that User1 has shared Project1 and all its child Artifacts granting User2 READ permission. Later User1 creates a new Experiment (Experiment 3) which is nested under Project1. User2 should have READ access to the new Experiment 3, even though it is created after Project1 was shared. To achieve this, Experiment 3 should inherit all the Sharing rules from its parent that are cascadable at creation time. To determine whether a sharing rule is cascadable we maintain a CASCADE field in the Sharing rule.

The model also provides the capability to revoke already defined sharing rules. This operation corresponds to the deletion of the specific Sharing rule. But some complications may arise in the case of cascading sharing rules when multiple inheritance yields the same Permission. For example, assume Experiment 1 and its child artifacts are shared with User2 with READ permission. This allows User2 to READ the File1. The corresponding entry in the Sharing can be written as:

```
INSERT INTO SHARING(ACTOR, ARTIFACT, PERMISSION, CASCADE)
VALUES(User2, File1, READ, True)
```

If User1 later decides to Share the Project1 and all its child artifacts with User2 with READ permission, this Sharing rule will also enable User2 to READ File1. But note that the corresponding Sharing rule entry for Experiment1 and File1 will be the same as in the previous case. This will either duplicate the Sharing rule or would not make any changes, based on the implementation. Later if User1 wants to revoke the Sharing defined on Experiment1, all the Sharing rules that were created as a result of that Sharing have to be deleted as per the following operation.

This will end up having only one Sharing rule allowing User2 to READ and Project1 and nothing else. Hence it is important to capture the inheriting parent Artifact when recording cascading Sharing rules and at the revocation time deleting only the ones that correspond to the specific revoking parent Artifact. The modified Sharing operation on Project1 will now look as follows.

Going back to our first scenario, granting User2 with READ permission on Project1, we could have achieved this in two other ways. One approach would be to use the Permission type hierarchy and Share Project with a Super permission of READ (e.g). An actor who has OWNER Permission on an Artifact will also have READ Permission. The other approach would be to Share the Artifact with an Actor that contains the User2. For example if Project1 is Shared with Group1 with READ Permission, then User2 will also have READ Permission on Project1 as a result of being a member of Group1. Similar to handling nested hierarchies in Artifacts, the nested hierarchies in Permission types and Groups can be handled either implicitly or explicitly. The implicit approach will record only the original Sharing rule and will defer the computational heavy lifting to the inference time. On the other hand, in the explicit approach, additional records will be created to each nested element. For example when Sharing with OWNER permission additional records will be created to READ and WRITE permission. However we found that most of the Permission Type and Group hierarchies in our use cases are short and flat and always will

be of cascade type (e.g. when sharing with a group it is always implied that it is sharing with all the nested members). Therefore the overhead of using the implicit approach is not significant. Hence we decided to use the implicit approach to handle Permission type and Group hierarchies.

Check Permissions: In our model, inference operations become straightforward and less costly because we put most of the computational heavy lifting on the sharing and revoking operations. The Check Permissions operation determines whether a specific Actor has a specific Permission to a specific Artifact. For example, consider the case where we want to determine whether User2 has READ Permission to Project1. In our model, which implicitly captures nested aspects in Permissions and Groups, we need to first find all the Permissions which subsume the READ permission and all groups that have User2 as a member. After finding those, Check Permissions can be easily executed as follows.

Get all Accessible Actors: Sometimes it is useful to view a list of Actors who have Permission to READ or WRITE an Artifact. For example, the Owner of an Artifact may want to review the current list of Actors before granting or revoking sharing permissions. To get the list of Actors we create a relational join between Actors and Sharing entities and then use a filter operation to retrieve the list of Actors who have a particular Permission to an Artifact. For example, the operation to find out the list of Actors who has READ permission to Experiment 1 can be executed as follows:

```
Permissions := READ.getSuperPermissions()

Permissions := Permissions U READ

SELECT ACTOR AS A FROM SHARING JOIN ACTOR WHERE SHARING.

PERMISSION IN Permissions AND SHARING.ARTIFACT =

Experiment1

Return A
```

Search/Browse: In the search operation, the objective is to retrieve a list of Artifacts that are accessible to a specific Actor based on some permission criteria and that conforms to a particular search criteria on Artifact properties. Browse is special case of search with empty Artifact filter criteria. As a practical requirement, when dealing with large return lists, it is also important to handle pagination. As the objective of this operation is to retrieve the list of Artifacts we do a relational join between Artifact and Sharing entities and then apply the filter criteria. In the current implementation, the Artifact filter criteria can be applied on Artifact name, description, owner, parent artifact (if exists), created and updated times and the full text field. Some of the example search/browse queries will be as follows:

- Browse without Artifact type constraint: e.g. Select Artifacts where User2 has READ access.
- Browse with Artifact type constraint: e.g. Select Artifacts of type EXPERIMENT where User2 has RE AD access.
- Search with Artifact filter criteria: e.g. Select first 10
 Artifacts of type EXPERIMENT where User2 has R
 EAD access and the Artifact name contains "Ethylbenzene" and Artifact created during last week.

The last search operation listed above can achieved as follows:

Groups := User2.getAllMemberGroups()

Groups := Groups U User2

Permissions := READ.getSuperPermissions()

Permissions := Permissions U READ

SELECT ARTIFACT AS A FROM SHARING JOIN ARTIFACT WHERE
SHARING.ACTOR IN Groups AND SHARING.PERMISSION IN
Permissions AND ARTIFACT.TYPE = EXPERIMENT AND ARTIFACT
.NAME CONTAINS EthylBenzene AND ARTIFACT.CREATED_DATE
IN LAST_WEEK LIMIT 10 OFFSET 0

Return A

5 INTEGRATION WITH SEAGRID

SEAGrid provides a traditionally secure data model where all the data has been considered to be proprietary and data sharing occurs only outside the SEAGrid application. However, recently users have requested the data be made shareable among collaborators to improve organization, post-pro cessing and collaborative discovery. The discovery and sharing of the data go hand in hand as the simulation data accumulates over time and data location and identity need to be maintained to reuse the same in subsequent simulations. Supporting data discovery by individual users and collaborative processing of data requires both metadata generation and data indexing. The original SEAGrid infrastructure provided a way to define key value pairs so users can manually add to a metadata catalog for each experiment they set up, along with a search engine to discover the tagged data and products. However, users did not adopt this system, as it required a disciplined addition of metadata tags.

Recently we eliminated the manual tagging operations by implementing an automated parsing and indexing system. This system generates metadata tags for output of some of the applications used in the SEAGrid gateway [10]. The parsing infrastructure created for the SEAGrid gateway provides access and discovery of any data shared with the user, as it becomes part of the searchable domain. Additional sharing infrastructure requires to define what is shared and with whom and a way to collaboratively process data. Toward this end SEAGrid have prototyped integrating Jupyter notebooks in a GSOC project that can be integrated into Apache Airavata gateway infrastructures to interact with data products with ready analysis functions available in Python [2].

The users have benefitted from the job history organization already available in the portal but were unable to exploit the vast amount of past data from the community as there was no infrastructure to share the data securely. SEAGrid now working on providing a generic way to publish data to community organizations such as Figshare or SeedMe.org, but more controlled sharing for collaborative and cooperative post-processing will require additional infrastructure to define collaborating individuals or groups, modes of sharing, and timelines. Sharing of post-processing functions/applications along with the data and/or provenance details would also be beneficial for reproducing data products as well additional enhancement to the analysis if needed. In addition to the data sharing requirements, SEAGrid may have to restrict resources such as applications due to accessibility to license, something that is being tested by a PI or one based on a restricted hardware resource such as campus/institutional resource. The group and sharing infrastructure need to support these modalities as well.

6 INTEGRATION WITH THE CIPRES WORKBENCH FRAMEWORK

The CIPRES Workbench Framework [8] was created with the assumption that each authenticated user was working independently of all others, which is consistent with the work paradigm of biological science when the software was designed. The software at present does not support collaboration or data sharing between individual accounts. However, recent surveys show that users of the Neuroscience Gateway (NSG) and the CIPRES Science Gateway, two highly accessed gateways built using the CIPRES Workbench framework, have a strong interest in sharing data within their workgroups, and with the public as well. Both user groups indicate that data access and data sharing present a significant challenge, and that users would appreciate a solution that can be managed from within the Gateway interface. Two specific use cases highlighting the data sharing needs of typical Workbench Framework users are listed below:

A geographically distributed, highly interdisciplinary neuroscience research group is interested in collaboration that combines empirical results from magnetoencephalography (MEG) experiments with detailed computational models of neocortical circuitry to infer the mechanisms responsible for generating cortical rhythmic activity. Experimental data is collected from geographically distributed collaborators' institutions, yet jointly all of them are developing a large-scale model of thalamocortical circuitry with detailed neurons and synaptic architectures and plan to run on supercomputers. Model predictions will be validated and informed with simultaneous thalamic and cortical microelectrode recording data (that needs to be shared) obtained in the collaborators' lab in other institutions in US and France [5].

EEGLAB [5] is a widely used software for processing experimental eletrophysiological (EEG) data by thousands of cognitive neuroscientists worldwide. Researchers are now interested in meta-analysis of source-resolved EEG measures across studies. This will allow research results of individual researchers/labs to be analyzed/compared (meta-analysis) to gain deeper understanding of brain functions at a higher



Figure 4: Mock user interface listing sharing summary

level. To be able to do this researchers will need a mechanism, within NSG, where they can make their data shareable such as by tagging results that they want to share with other researchers or make it public. This will require different level of sharing capabilities. This will then allow other researchers to perform meta-analysis of research results at a higher level using computing power provided by NSG.

Based on user feedback and the use cases above, tools for sharing data between accounts are a priority feature for CIPRES Workbench users. Accordingly, we are integrating the data sharing service with the CIPRES Workbench framework. Our approach will take a somewhat different strategy from the SEAGrid integration described above. For the Workbench Framework, a separate group management server will allow users to perform group and user management. This will allow full access to all group/user management functions in the Science Gateway Platform as a Service (SciGaP) sharing service without requiring any User Interface development. The CIPRES Workbench will retain an internal representation of Experiment configuration, so the shared Entities will be project folders. Within the Workbench code, project folder identifiers will be used to determine user access to contained Data and Experiments (Tasks in workbench terminology). Integration with the Experiment Catalog will not be required.

In the implementation for CIPRES and NSG, users will be able to access shared folders and control access to their experiments and data through the browser interface of the respective applications. Authenticated users can configure sharing/display preferences for their account profile. Folders (Artifacts) the user creates can be configured individually for sharing with Users or Groups. Figures 4, 5 and 6 illustrated the mocked interfaces of these features being built over Apache Airavata's Sharing Service. The new interface will also provide users with the ability to check, set, and revoke sharing permissions on Artifacts they create. For data shared with the user, a "shared data" folder will appear in the user interface. Users can view shared Files, Experiments, and Projects. In our initial implementation, read-only Artifacts can be cloned from the shared folder, and then can be

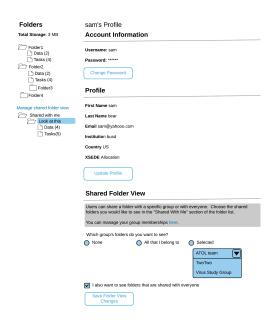


Figure 5: Mock implementation to choose a selected user or group to share a folder

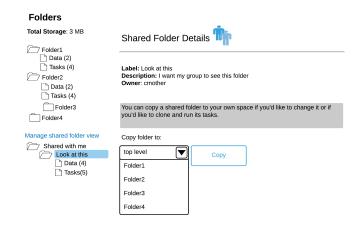


Figure 6: Read only permissions of a shared folder alerts the user to clone but not write into it

modified and resubmitted; the cloned jobs will be owned by the submitting user.

7 RELATED WORK

Internet2's Grouper [1] is an access management system that is widely used in universities that can support most of the required features in our proposed solution. Grouper provides comprehensive and efficient group management functionalities including rule and time based group membership definitions and ability to define groups based on complex group math operations (unions, intersections and differences) that are generally beyond the simple group management requirements in gateways. Features in Grouper such roles, attributes, and permissions can be used to implement our sharing model.

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If implemented using Grouper, the system can easily support the sharing and revoking of Artifacts, check permission, and get all accessible users operations. However the lack of flexibility in the Grouper's search/browse APIs hinders the system in efficiently fulfilling the search/browse operations required by the Gateways users. Search/Browse operations are an important aspect for Gateways, as we have described.

SeedMe [4] is a cyberinfrastructure platform that enables seamless sharing and visualization of computer simulation outputs which runs on HPC infrastructures through a web based tool. It enables users to conveniently view and access simulation outputs. Users can create collections of data items and share publicly or with a specified group of users. In the current implementation it has a single permission level, which grants permission to shared users to view and comment on the collection. Also it lacks the ability to define reusable user groups and requires explicitly defining the list of users every time when sharing a collection.

Globus Groups [3] can be used for access control by other Globus services, and are especially useful for file sharing. In the case of file sharing, file should first make it accessible as a Globus shared endpoint by configuring a Globus connect server. Then the owner of the file can share it with individual Globus users or Globus groups either with READ or WRITE permission. However it does not provide the functionality to create arbitrary Artifacts and share it with others.

8 CONCLUSIONS

In this paper we have presented a generic software design for the implementation of collaboration capabilities in Science Gateways. As the adoption of gateways accelerates, collaboration amongst users becomes second nature and an expected feature. Such new capabilities not only multiply the impact of these infrastructures but provide maximum use of computational resources.

The key contribution of the paper is to foster user collaborations based on group memberships. The paper discusses the underpinning architectural concepts, a relational data model in which the relationship between groups, permissions and resources are flexibly defined and managed. We further discussed the implementation of these concepts to meet the 4 key gateway requirements of Sharing and Revoking; Checking permissions; Browsing and Searching across all accessible entities. We further discussed the integration with SEAGrid gateway and evaluations by CIPRES and NSG Science Gateways.

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