THE NATIONAL FUSION COLLABORATORY PROJECT: APPLYING GRID TECHNOLOGY FOR MAGNETIC FUSION RESEARCH

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The overall goal of the DOE SciDAC funded U.S. National Fusion Collaboratory Project (http://www.fusiongrid.org/) is to improve the productivity of fusion sciences research through the development and deployment of advanced software tools that reduce the technical barriers to collaboration and sharing on a national scale. Our vision is to make resources—data, computers along with analysis, simulation and visualization codes—widely and transparently available as network accessible services, thereby enabling real-time multi-institutional collaboration on fusion experiments and improving comparisons between experiments and theory. The project unites fusion and computer science researchers to develop and deploy a national Fusion Energy Sciences Grid (FusionGrid), a system for secure sharing of computation, visualization, and data resources over the Internet. Some of the early prototype FusionGrid services proved so successful they are now used in a production environment for everyday fusion research. The success of other prototype services has resulted in fusion research funds being used to purchase necessary hardware to create production services. Future work is planned to augment the services currently available with FusionGrid, transition prototype services to production capability, and put in place the infrastructure to support a larger user base.

1. Introduction

Developing a reliable energy system that is economically and environmentally sustainable is the long-term goal of Fusion Energy Science (FES) research. As fusion experiments have increased in size and complexity, there has been a concurrent growth in the number and importance of collaborations among large groups at the experimental sites and smaller groups located nationwide. Teaming with the experimental community is a theoretical and simulation community whose efforts range from applied analysis of experimental data to fundamental theory (e.g., realistic nonlinear 3D plasma models). As a result of the highly collaborative nature of FES research, the community is facing new and unique challenges.

Deployment of the prototype and production FusionGrid infrastructure [1,2,3] has been made possible through work supported by the DOE SciDAC program and from base funding for FES research. Substantial progress has been made in deploying FusionGrid. The TRANSP code [4], used for time-dependent analysis and simulation of tokamak plasmas, has been released as a remotely accessible FusionGrid computational service along with supporting infrastructure development (data storage, monitoring, user GUI) [5]. This

FusionGrid service has been so successful that it has become the production system for TRANSP use in the United States and is starting to be adopted internationally. The Access Grid (AG) [6] has been deployed and used at major fusion experiments in support of remote participation. Furthermore, progress has been made in shared applications and displays with testing and user feedback that has helped sharpen the requirements for a truly collaborative control room for fusion experiments.

To dramatically affect the efficiency of experimental FES it is necessary to combine Grid computing with unique collaboration technologies such as the AG and application sharing. The combination of these technologies into a unified scientific research environment is a demanding and unique challenge and is outlined in the paper that follows.

2. FusionGrid: Requirements and Challenges

The vision for FusionGrid is that experimental and simulation data, computer codes, analysis routines, visualization tools, and remote collaboration tools are to be thought of as network services. In this model, an application service provider (ASP) provides and maintains codes as well as resources that those codes would execute on. This mode of operation has advantages for both the client and the provider: it frees the clients from maintaining and updating software and the providers from porting and supporting it on a wide range of platforms. In this environment, access to services is stressed rather than data or software portability. Consequently, FusionGrid is not focused on utility computing (e.g., SETI@home) or distributed supercomputing that are typical justifications for Grid computing, but simply on making the ASP paradigm effective for Grids.

The ultimate goal of FusionGrid is to allow scientists at geographically distributed sites to participate fully in experimental and computational activities, whether by code execution or personal participation, as if they were working at a common site. We call this vision the collaborative tokamak control room and expect that it will dramatically increase the productivity of experimental science.

The collaborative control room is centered on the cyclical nature of experimental fusion research (Fig. 1). In any given day, 25–35 plasma pulses are taken with approximately 10 to 20 minutes in between each ~10 second pulse. For every plasma pulse, up to 10,000 separate measurements versus time are acquired at sample rates from kHz to MHz, representing about a gigabyte of data. Throughout the experimental session, hardware/software plasma control adjustments are made as required by the experimental science. These adjustments are debated and discussed among the experimental team. Decisions for changes to the next pulse are informed by data analysis conducted within the roughly 20-minute between-pulse interval. This mode of operation places a large premium on rapid data analysis that can be assimilated in near-real time by a geographically dispersed research team. To be fully functional, the collaborative control room requires (1) secured computational services that can be scheduled as required, (2) the ability to rapidly compare experimental data with simulation results, (3) a means to easily share individual results with the group by moving application windows to a shared display, and (4) the ability for remote scientists to be fully engaged in experimental operations through shared audio, video, and applications.

Data analysis to support experimental operations includes between pulse analysis of raw acquired data as well as the merging of numerous data sources for whole-device simulation of the experimental plasma. Results of more detailed, computationally demanding predictive simulations, carried out during the planning phase prior to the experiment are made available for comparison to the actual experimental results in real time. FusionGrid-based computational services in support of experimental operations have the potential to greatly enhance the quantity of data analysis and the quality of experimental science. Additionally, this same FusionGrid architecture can support other, more computational demanding services

that are not candidates for between-pulse data analysis. Therefore, fusion scientists can learn to use the Grid for all computational requirements.

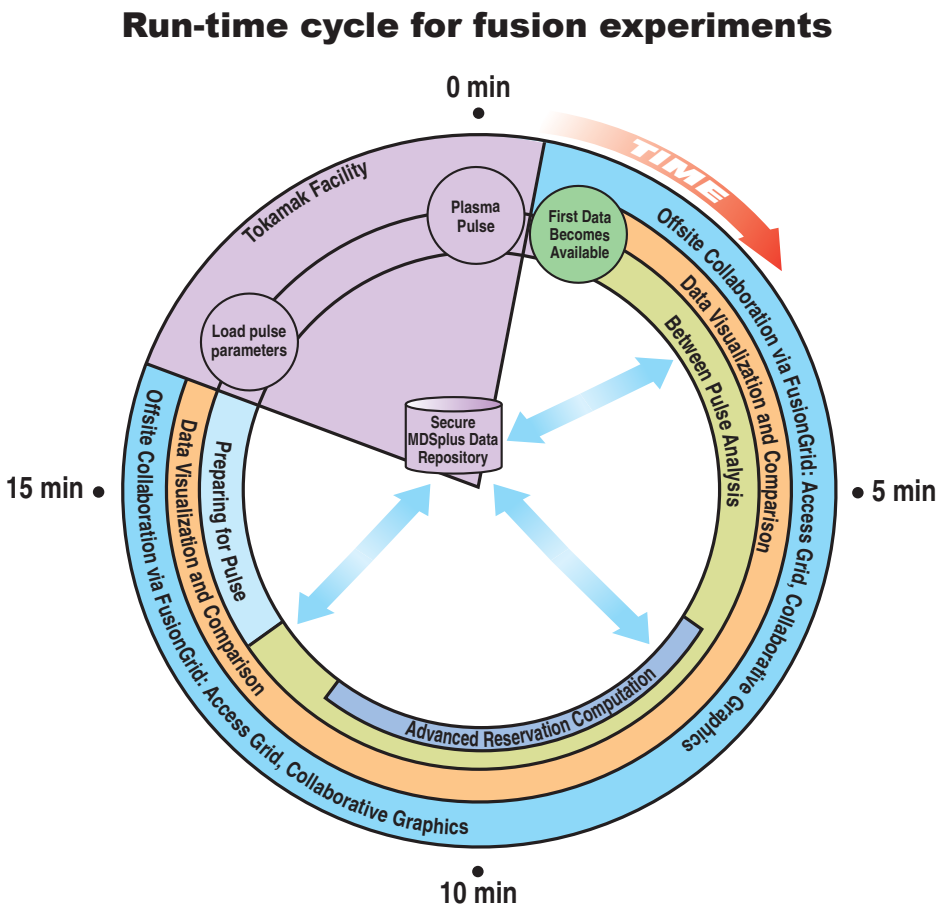

Fig. 1. Experimental magnetic fusion is cyclical in nature with fusion plasmas produced approximately every 20 minutes. Machine control is physically located on-site, but other work can be done off-site as appropriate. The collaborative control room will allow the integration of off-site tasks into experimental operations.

In addition to technical challenges, the most serious challenges to implementing FusionGrid on a large scale are issues of usability and deployment. In deployment, firewalls are currently our most serious issue. Firewalls and related security measures are typically not a matter of choice for the involved institutions. The introduction of firewalls in the fusion labs was mandated by DOE order 205.1 in answer to security violations at the labs. Utilizing GT2-based services on a firewall-protected site requires the opening of a number of static ports, and, more significant, an unpredictable number of dynamically chosen ephemeral ports created only for a specific session. Although some of these problems are resolved in GT3, some problems persist. Most important, users have found that the additional authentication required by firewalls with SecurID obviate the single sign-on advantage to Grid computing.

3. Grid Technologies in FusionGrid

To be successfully deployed, FusionGrid requires a broad range of components including underlying Grid tools and human-computer interfaces that makes its use straightforward for fusion scientists. Grid tools needed include those supporting user and resource authentication; distributed authorization, resource management, and enforcement tools (to give

stakeholders control of real and intellectual property); secured shared computational services; shared applications and displays; and high-quality, flexible audiovisual applications.

3.1. Tools

FusionGrid creates a virtual organization of the U.S. fusion community whose resources are protected by a shared security infrastructure based on authentication as well as authorization to allow fine-grained control of codes and resources. Authentication is based on X.509 identity certificates issued by the DOE Grids Certificate Authority (CA) as the global identifier for FusionGrid members. The Globus Toolkit® (GT2) is employed by FusionGrid to provide secure authentication, remote job execution, and communication over the open Internet. Of particular benefit to the user community is the single sign-on capability, since they need only log-on once, no matter how many services they use. GT2 is also used for starting remote computation and secure data transfer between fusion codes and databases.

In order to enable controlled resource sharing, an authorization callout was implemented in GT2 that enforces job creation as well as management decision [7,8]. After evaluating a job creation request specified in GT2's Resource Specification Language (RSL) in the context of authorization policies, an authorized user is allowed to create a job that can then be managed by another authorized user according to agreed-upon polices. These policies are expressed in and evaluated by the Akenti authorization system [9] called from the Globus Toolkit [10]. A production version of the GT2 callout has been released and is being deploying on FusionGrid.

To provide a better form of enforcement for authorization policies and to alleviate the administrative burden on the administrators of fusion sites, we have developed a prototype dynamic account management system [11]. It allows a user, authorized by its Grid identity, to create a local account on a resource for a limited time, and later manage that account, again based on authorization. Although this infrastructure has not yet been integrated with an authorization system and used in production, the prototype code for dynamic accounts is currently available [12].

In order to enable the between-pulse execution of analysis and simulation codes an agreement-based system has been developed to provide end-to-end agreements on between-pulse code execution. This system combines resource reservations [13] with application runtime and data transfer prediction to provide advance estimates of execution times and the level to which its completion can be guaranteed. This work has contributed to the development of WS-Agreement at the Global Grid Forum (GGF) and has been demonstrated at SC03. While the GT2 implementation of the Globus Toolkit is used in the production FusionGrid, dynamic accounts prototype and between-pulse code execution are being developed in GT3.

Data access on FusionGrid has been made available using the MDSPlus data acquisition and data management system [14], by far the most widely used and successful data acquisition and management system in the international fusion community. MDSplus provides a convenient metadata representation and layer facilitating fusion data management. MDSplus communication has been layered on top of the Globus IO to take advantage of the Globus Security Infrastructure (GSI) and create secure data access on FusionGrid using the standard MDSplus interface without any loss in speed or functionality. At present, the three main MDSplus experimental data repositories at Alcator C–Mod, DIII–D, and NSTX are securely available on FusionGrid. Data management by MDSplus of large datasets generated by simulation codes is being tested. All access to relational databases, which are widely used in the fusion program and typically run on Microsoft Windows platforms, is currently done insecurely through MDSplus because a production version of the Globus Toolkit for Windows is unavailable.

With multiple applications distributed throughout a Grid infrastructure, it becomes a challenge to monitor the progress and state of each application. Users of a Grid environment

need to know the specific state of code runs, when their data results are available, or if the requested application is even available. To track and monitor applications on FusionGrid, the FusionGrid Monitor (FGM) has been developed as a Java servlet that can accept and monitor information from remote and distributed applications [15]. Currently, FGM tracks TRANSP analysis runs on the National Fusion Grid and provides updated information on each individual run, including current state, CPU time, wall time, comments, and access to log files that have been produced by the analysis. The Fusion Grid Monitoring system has built to provide user output through HTML, utilizing both server push and client pull capabilities. This allows multiple users to connect to FGM, view their code runs by using a web browser, and obtain updated information without excessive user input or client software. Designed in the Java language, the monitoring system is portable; and with the inclusion of the Java Expert System Shell (JESS), the system is also expandable and customizable. Online access to log files is available through FGM, using anonymous FTP.

The Access Grid is used by FusionGrid to create a service that enables group-to-group interaction and collaboration that improves the user experience beyond teleconferencing. The Access Grid provides scientific research with a complex multisite collaborative experience integrated with high-end visualization environments including tiled display walls [16]. To meet the needs of the FES research community, the Personal Interface to the Grid (PIG) was developed, offering a low-cost alternative to a full-scale conference room size AG node. Currently, PIGs are installed at C–Mod and DIII–D and a full-scale AG node at PPPL. Most important, a PIG was also installed in the DIII–D control room and was used in a joint experiment between C–Mod and DIII–D. The initial test proved valuable in terms of the potential for such collaboration, and we plan to make such collaboration standard.

To enhance collaboration, in addition to Grid technologies we are using visualization technology. Tiled display walls are being used to enhance the collaborative work environment of the tokamak control room (Fig. 2). Software tools and techniques, such as work on improving data distribution and scalability, are being developed to increase their ease–of–use in these environments. For example, as a prototype FusionGrid service, remote collaboration between two geographically separated tiled walls with networking software has been prototyped to form a shared collaborative display. We are also using the SCIRun problem solving environment for advanced scientific visualization. Such a capability allows for the exploration of complex simulation results and the comparison of simulation and experimental data within the collaborative control room.

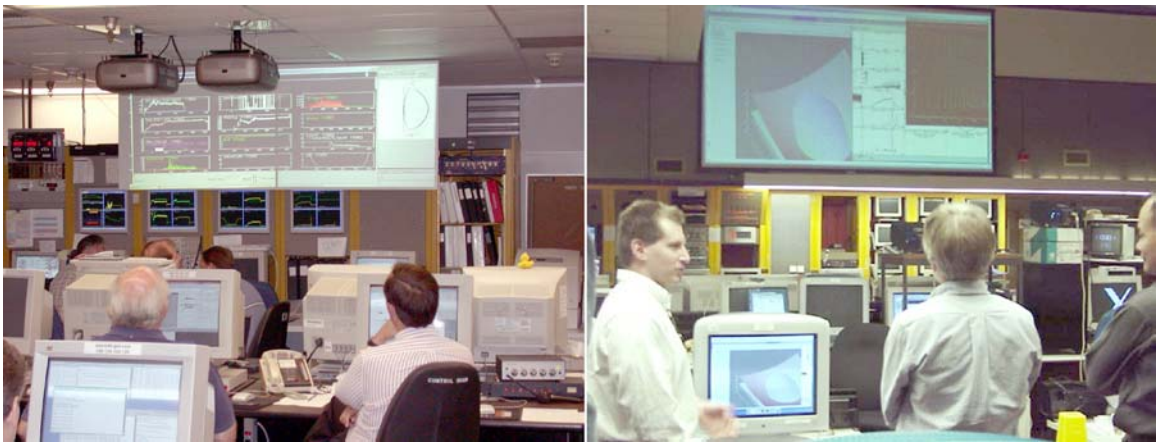

Fig. 2. The collaborative fusion control room has been tested during experimental operations. DIII–D (San Diego) is on the left and NSTX (Princeton) is on the right.

3.2. Interfaces

3.2.1. User Interfaces

Fusion scientists manually manage their identity certificates using the DOE Grids certificate management system. Both the NFC project team and fusion scientists found the process to be cumbersome, especially for new users. Typically, researchers request a long-term certificate through their Web browser, export the PKCS#12 file, transfer the file from their desktop computer to a UNIX host, use OpenSSL utilities to extract the private key and certificate from the PKCS#12 file, then install those files in the expected directory under the correct permissions. This multistep complex process is a serious usability issue and prevents widespread adoption of FusionGrid. A myProxy server [17] will be prototyped as a solution by storing the user's long-term credentials on a secure host. The standard grid-proxy-init command will be supplemented with a command that will retrieve a proxy certificate from the myProxy host. The long-term certificates will be password protected.

For ease of use, a GUI utility called PreTRANSP was created for input data preparation and TRANSP code innovation. PreTRANSP serves as the primary interface to Grid-enabled TRANSP and is written in the Interactive Data Language (IDL). PreTRANSP assigns unique run id numbers to new TRANSP runs, allows researchers to search through existing runs, loads inputs, sends messages to the monitoring system, and submits TRANSP jobs for remote execution using the Globus Toolkit. All of these activities either happen behind the scenes or are controlled by the user through the PreTRANSP GUI. For example, the mechanism for submitting a TRANSP job for execution is a large, friendly start button.

TRANSP monitoring information is displayed through the Fusion Grid Monitor (FGM). The FGM uses server-push technology to update client web browsers when new monitoring information has been posted by TRANSP. TRANSP users can monitor the status of their code runs, view log files through an anonymous-FTP mechanism, and plot results as they are being calculated, all through the FGM. The log files are processed server-side. The plotting feature is handled through ElVis, a Java applet that runs client-side. We find this Web-based interface to be very convenient.

Currently there is no user interface for editing and managing authorization policies governing access to TRANSP. FusionGrid has prototyped authorization using Akenti, but is currently not using this feature in production. Our current focus is on developing good policy management tools allowing a service administrator easy understanding of policies and quick reaction to policy changes. This is of particular importance because we anticipate that authorization will become increasingly important as the number of services grows.

3.2.2. Software Interfaces

The PreTRANSP client described in the preceding section relies exclusively on Globus Toolkit command-line tools such as globus-url-copy, and globus-job-submit to manage interactions in the Grid. Secure MDSplus, whose interactions are more tightly coupled, leverages the globus_io and globus_common modules that ship with the Globus Toolkit. The result is that Secure MDSplus can securely transfer data with no loss of performance relative to normal MDSplus. We are awaiting the release of XIO features that will allow us to incorporate more advanced communication capabilities.

TRANSP calls secure MDSplus using the standard MDSplus C API routines such as mdsconnect and mdsvalue. TRANSP is linked against secure MDSplus, and by extension the Globus Toolkit shared libraries, at compile time. Again, this tight coupling results in efficient data transfer, an important feature for large scientific codes.

Currently, SQL Server is accessed through MIT-written IDL procedures that use call_external. This connection is not encrypted and uses only the standard SQL Server security features. Since a release of Globus for Windows is not available, secure database connections are possible only through the use of an intermediate secure MDSplus server. This intermediary scheme was tested and works well enough, but performance is not as good

because of the intermediate step. When the intermediate secure MDSplus server runs on the SQL Server host, memory allocations are greatly increased since—whether one uses client-side or server-side cursors—at least one cursor will be running on the server machine in the intermediary. If the intermediary runs elsewhere, then the network hops are increased, and the intermediary-SQL Server connections are left unencrypted.

3.3. Performance Considerations

Two performance considerations have become apparent with the initial deployment of FusionGrid. The first is the performance slowdown resulting from WAN latency of many data transactions per TRANSP computation. The input and output data for TRANSP is not large in total, but there are on the order of 1000 different quantities to move over the WAN via MDSplus. For between-pulse data processing and digesting of results by the experimental team, the slowdown was unacceptable. Instead, the individual quantities were packaged in one file for WAN transfer. The second is the performance slowdown associated with application sharing with remote users. Initial feedback from testing indicates that on-site personnel consider the present slowdown unacceptable. Work continues to quantify both of these performance issues and investigate methodologies for overcoming the limitations.

4. FusionGrid Applications

The code TRANSP, used for time-dependent analysis and simulation of tokamak plasmas, was released in late 2002 as a service on FusionGrid. Running on a Linux cluster at Princeton Plasma Physics Laboratory (PPPL), this FusionGrid service has performed over 1,500 simulations taking over 10,000 CPU-hours for 9 different experimental fusion devices (Fig. 3). Both the input data and output data of TRANSP are securely written and read from an MDSplus and SQL data repository. Monitoring and tracking of these runs have been accomplished through the deployment of the FusionGrid Monitoring System (FGM), a derivative of the Data Analysis Monitoring System used at DIII–D.

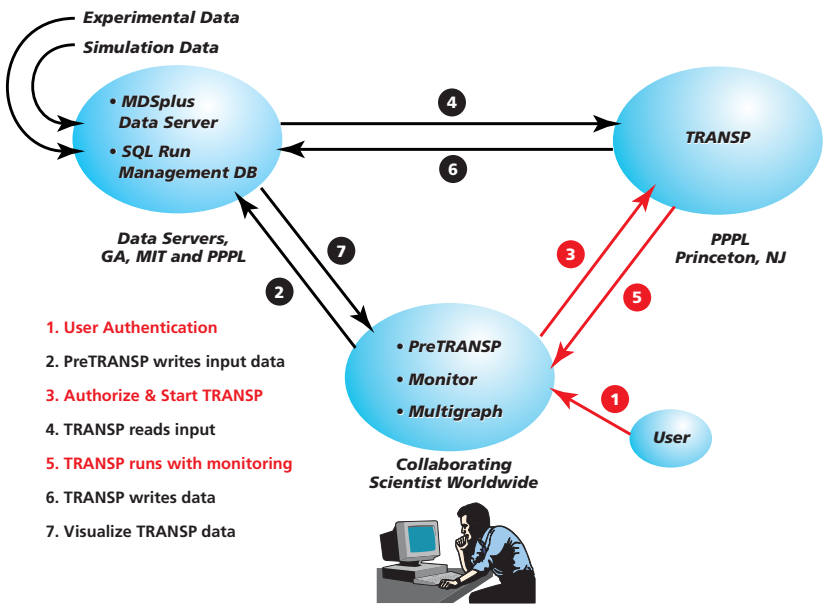

Fig. 3. TRANSP as a FusionGrid service based at PPPL is securely available from anywhere in the world.

Deployment of TRANSP on FusionGrid frees scientists from the need to build and maintain local versions of a large and complex code and, at the same time, eases the burden on the code development team, which was previously required to provide support on a highly heterogeneous set of remote machines. Further, the Grid implementation enabled users to perform significantly more calculations, resulting in more rapid progress than prior to the deployment of FusionGrid. Scientific results using FusionGrid were presented at the 2002 and 2003 American Physical Society Division of Plasma Physics (APS/DPP) meetings and the 2002 19th IAEA Fusion Energy Conference. The service proved extremely popular in our community with at present approximately 50 FusionGrid users with several based in Europe.

In a similar manner in which the Globus Toolkit was combined with fusion science-specific tools and interfaces to release the TRANSP service, the AG node has been combined with fusion-specific displays and application sharing to create the service for remote experimental participation. In order to be effective, remote participation must include real-time information to yield a sense of control room presence. This is critical for off-site scientists to effectively participate in an experiment and must include all real-time data displayed to on-site staff. Sense of presence includes the ability to see and hear what people see and hear in the control room. Even more important to a remote collaborator is the information flow throughout the twenty-minute pulse cycle. This information includes the pulse cycle/status clock, pulse parameters, status of between-pulse analysis, and announcements from the scientist in charge.

The FusionGrid requirement for researchers to remotely participate in experimental operations has been tested with the desktop AG node combined with the ability to share applications. Additionally, real-time control room information is currently made available to remote participants through a fusion-specific Web interface. The tokamak control computer has the pulse cycle information and plasma control parameters. While it sends the information to the large LED display in the control room, it also writes the same data directly to a Web server that parses them into a reasonable format for display on the Web page. The Web client checks with the web server periodically and updates the status accordingly. Integrated in the same display is a quick view of the data acquisition and analysis status. Whenever a group of data becomes available, the corresponding indicator changes color. The statuses are made available by the MDSplus event system that drives the analysis cycle. Therefore, remote scientists can combine the AG node, shared application, and Web display for a full sense of control room presence, resulting in their complete integration into the decision-making process of the experimental control room.

5. Lessons Learned

The real-world use and testing of FusionGrid services have highlighted several areas where additional work is required before large-scale adoption is undertaken in the fusion community. First and foremost, the management of certificates has to be made simpler and easier for both the service user and the service provider. A researcher's first experience with FusionGrid is obtaining and installing a X.509 certificate. Present difficulties must be resolved so the scientist's first impression will be positive.

The conflicting requirements of Grid computing and site security (firewalls) makes expansion of FusionGrid services a time-consuming task and one that does not scale to over 1,000 U.S.-based scientists. To avoid excessive exposure by opening the firewall, site administrators will often open ports only to specific IP addresses (insufficient to support dynamic client access in the Grid) or use it in conjunction with other technologies, such as SecurID. The use of SecurID allows for more flexibility because a session is established based on a token and then the firewall is dynamically modified to open a set of ports for traffic coming from the IP that established the secure session. The ports that get opened are defined in the profile of the user (negotiated out of band) who established the secure session.

Although more flexible than relying on static firewall configuration, however, the SecurID solution has its own problems. The ports get opened for a fixed, preconfigured time only. After that time the secure session is terminated and can be reestablished only manually, a process that results in termination of all existing connections and their state, thereby terminating an existing Grid session. A more serious problem is that every institution in a Grid will typically have its own SecurID system so that establishing connections to two institutions requires two SecurID cards, increasing the complexity the user needs to deal with. Clearly this type of independent SecurID system does not scale for a national deployment of FusionGrid.

Efficient data management of large simulation datasets is required so that rapid comparison of simulation data to experimental data is possible in the tokamak control room. In order to accommodate large-scale simulations, a new MDSplus server has been installed and configured at NERSC. Performance testing will start using the NIMROD code running on the Seaborg computer. Included will be tests of MDSplus I/O performance comparing local LAN and WAN connections using a variety of transport levels. Comparisons with other data transport mechanisms, notably HDF5 with GridFTP will also be carried out.

Initial testing and usage of shared applications in the control room identified efficiency issues that must be resolved before the capability is adopted for the control room. Feedback from scientists in the control room indicated that when they began sharing with remote users, they themselves began to feel as if they were remotely located because their computer response became significantly slower. Giving a remote scientist a new capability at the expense of on-site staff is not acceptable.

In the fusion control room environment, ambient audio can be distracting to a collaborative session; this reduces the effectiveness of the Access Grids audio system. Isolating the Access Grid users with headsets is one way to improve the audio provided by the Access Grid. This has two advantages. First, if there is no ambient audio output, the echo cancellation hardware is not needed, which saves cost. Second, it provides each user with a dedicated audio channel delivered directly to them, removing distractions from ambient noise. The disadvantage to this approach is it tethers the user to the desk and in the case of headphone-based systems inhibits the user's ability to interact with local collaborators. The possible of using Bluetooth headsets for providing individually delivered public audio channel has been proposed. This could form the basis for future work in private audio channels leading to the support of multiple audio channels within an Access Grid environment.

The increasing user base of FusionGrid combined with the addition of new services will require better education, training, and documentation. Users, developers, and systems administrators will need access to crucial information in order to make best use of FusionGrid. This information has been provided mostly by word of mouth by project members but this solution does not scale for a membership on the order of 1000. To be successful, a users guide, a developers guide, and an administrators guide will need to be created for FusionGrid.

6. Conclusion

The main thrust of future work for FusionGrid is aimed toward ease of use, including easier certificate management, easier and more uniform access into FusionGrid code services possibly via Web portals, and better interplay between FusionGrid security and site security (firewalls). At the same time, new code services will be deployed as requested by the user community. For FusionGrid's advanced collaboration service, the challenge is to develop a science of collaboration: to understand what works and why (human factors and social issues), what functionality is needed, and how should it be interfaced to the users as part of FusionGrid.

As Grid middleware evolves, there is a concern that trying to satisfy all possible Grid use scenarios will result in exceedingly complex software. Simple software that quickly allows users and service providers to join FusionGrid will be seen as an advantage; the benefit of joining far outweighs the time required to join. Maintaining tightly coupled software, at all levels, that contains only what is required will be the best way to ensure that FusionGrid evolves into a streamlined efficient system for the U.S. fusion community.

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