TeraGrid Science Gateways and Their Impact on Science

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The Science Gateways program seeks to provide researchers with easy access to TeraGrid's high-performance computing resources. A look at four successful gateways illustrates the program's goals, challenges, and opportunities.

Funded by the National Science Foundation (NSF), TeraGrid (www.teragrid.org) is one of the world's largest distributed cyberinfrastructures for open scientific research. The project began in 2001 as the Distributed Terascale Facility, which linked computers, visualization systems, and data at four sites through a dedicated 40-gigabit optical network. Today TeraGrid includes 25 platforms at 11 sites and provides access to more than a petaflop of computing power and petabytes of storage.

TeraGrid has three primary focus areas. Its *deep* goal is to support the most challenging computational science activities—those that cannot be achieved without TeraGrid facilities. TeraGrid's *wide* mission is to broaden its user base. The project's *open* goal is to achieve compatibility with peer grids and information services that allow development of programmatic interfaces to TeraGrid.

A part of TeraGrid's wide initiative is the TeraGrid Science Gateways program. To explain the program's conceptual basis and illustrate supporting services that have evolved within TeraGrid, we highlight four successful science gateways: the Computational Chemistry Grid (GridChem), Linked Environments for Atmospheric Discovery (LEAD), nanoHUB.org, and the Cancer Biomedical Informatics Grid (caBIG).

PROGRAM GOALS AND ORIGINS

The TeraGrid Science Gateways program began in late 2004 with the recognition that scientists were designing their own specialized user interfaces and tools to marshal digital resources. Much of this work was in response to the growth of the Web and increasing digital data available through sensors and large-scale computation. It became clear to TeraGrid's designers that providing scientists access to high-end resources such as supercomputers and data archives through application-oriented interfaces designed by science community members would make unprecedented capabilities available to researchers unfamiliar with the arcane world of high-performance computing.

Access to HPC resources has historically been restricted to students who work directly with a funded "principal investigator." Science gateways typically operate through direct Web access or downloadable client programs, greatly reducing the barrier to entry and encouraging exploration by a much wider set of researchers. This access brings the best minds, regardless of location, to bear on the most challenging scientific problems and encourages individuals with a new perspective to become involved.

With an increasing set of problems requiring cross-disciplinary solutions, gateways can clearly have a major impact on scientific discovery. And because stu-

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dents can participate regardless of their institutional affiliation, gateways can increase participation among underrepresented groups and contribute to workforce development.

SCIENCE GATEWAYS

A science gateway is a framework of tools that allows scientists to run applications with little concern for where the computation actually takes place. This is similar to cloud computing in which applications run as Web services on remote resources in a manner that is not visible to the end user. However, a science gateway is usually more than a collection of applications. Gateways often let users store, manage, catalog, and share large data collections or rapidly evolving novel applications they cannot find anywhere else. Training and education are also a significant part of some science gateways.

The level of cloudlike abstraction and virtualization varies from one gateway to another as different disciplines have different expectations regarding the degree to which its users require the underlying TeraGrid resources. Usually, a gateway has a core team of supercomputing-savvy developers who build and deploy the applications that become services available to the community at large. One of the Science Gateways team's primary jobs is providing tools and services for these core developers.

TeraGrid currently provides back-end resources to 29 gateways that span scientific disciplines and technology approaches.

Other gateways focus on services' broad-based usability; they spend significant effort creating friendly GUI technology and smoothing the transition of data between various computational resources. Delivery of computing cycles to users rapidly and interactively without any specific grid knowledge is critical.

TERAGRID GATEWAY SUPPORT

TeraGrid currently provides back-end resources to 29 gateways that span scientific disciplines and technology approaches. Various research communities independently develop these gateways to meet defined objectives. TeraGrid, however, must develop scalable service solutions to meet the myriad needs that result from this decentralized development.

Early in the Science Gateways program, TeraGrid leaders surveyed the researchers behind 10 gateways to better understand what common services this new user community required. Commonalities emerged in the areas of Web services, community accounts, auditing, a scalable and robust infrastructure, and flexible resource allocation and scheduling.

Web services

Some gateway developers rely on the convenience that Web services provide and have requested such capabilities. Version 4 of the Globus Toolkit (www.globus.org), installed across TeraGrid in 2006, includes Web service support for tasks such as job submission and data transfer. Approximately 25 percent of gateways use Web services.

Work continues to augment the basic functionality provided by Globus with TeraGrid-specific information. For example, job submission interfaces can include data used to answer questions such as "Where can I run my 16-processor job that requires 20 Mbytes of memory the soonest?" "Where can I run an 18-hour, 8-processor job using the computational chemistry code Gaussian the soonest?" "Which sites support urgent computing for a 32-processor job?" and "Do any of these selections change if a 25-Gbyte input file needs to be transferred to the site of interest?"

Because some gateways provide as well as consume Web services, TeraGrid is developing a registry where developers can list and share services with one another as well as with potential users. Today, researchers interested in using software on TeraGrid check a catalog that lists software available from the command line on all resource-provider platforms, but we envision future researchers and developers checking a registry of applications either programmatically or manually.

Community accounts

TeraGrid uses community accounts to delegate account management, accounting, certificate management, and user support directly to the gateways. To responsibly delegate these tasks, however, TeraGrid must provide management and accounting tools to gateway developers and store additional attributes for jobs submitted through community accounts. Some resource provider sites further secure these accounts by using the community shell, commsh.

Auditing

Soon after the Science Gateways program got under way, the Globus grid resource allocation and management project developed GRAM Audit, an extension that lets gateway developers retrieve the amount of CPU hours a grid job consumes after it has completed. With jobs for many independent gateway users running from a single community account, such a capability is quite important. The Science Gateways team is currently developing GridShib, a tool that lets gateway developers store attributes unique to a gateway user when jobs are submitted to TeraGrid. This will provide a programmatic way to count TeraGrid gateway end users as well as allow per-user accounting for gateways as needed.

Scalable and robust infrastructure

Supporting various gateways in an environment as extensive as TeraGrid requires a commitment to scalable infrastructure. For example, in 2007, students from numerous institutions used the LEAD gateway in a weather forecast competition. The nature of the competition led to concentrated bursts of job submissions and data transfer requests. During this period, the system was not as stable as hoped, resulting in an extensive collaboration between Globus members and TeraGrid staff to understand and address both the hardware and software issues associated with handling the large load.

In addition, there are sometimes unscheduled outages when using shared resources. Gateway developers must use fault-tolerant programming methods. As gateway use of TeraGrid expands, periods of high load will be even less predictable. This requires deploying a robust infrastructure, and developers must use failover models to ensure stable services. Addressing these issues continues to be a focus.

> **Supporting various gateways in an environment as extensive as TeraGrid requires a commitment to scalable infrastructure.**

Flexible resource allocation and scheduling

TeraGrid has had to adapt its allocation and scheduling policies to meet gateway needs. Because usage cannot be planned as it can with single investigators and their research teams, flexible allocation policies are required. When requesting resources, principal investigators must be able to describe in general terms how they expect their gateway to be used, and TeraGrid must be able to react if a gateway is more successful than anticipated. Avoiding service interruptions is likewise necessary to ensure continuity and reliability. Gateways also tend to have greater interactive needs than researchers working at the command line.

Gateway developers have been early testers in TeraGrid's metascheduling efforts. Their insight has led to development of the Special Priority and Urgent Computing Environment within TeraGrid to meet urgent computing needs, when simulations might be required immediately—for example, in response to sensor data feedback.

GRIDCHEM

Molecular sciences occupy a central position in material behavior research. Most physical phenomena, from atmospheric and environmental effects to medicinal interactions within cells, are mediated through forces at the molecular and atomic level. Nanodevice modeling and material design also involve atomic-level detail. Chemical, biological, and material modeling require access to unique and coupled applications to produce accurate and detailed descriptions of atomic interactions. The insights gained help researchers design novel and appropriate materials and devices for a given task.

The need for integrative services to drive molecular-level understanding of physical phenomena has become acute in an era of rapid prototyping of nanoscale actors, multidisciplinary engagement with chemical sciences, and diverse and complex computational infrastructures. Automated computational molecular science services will transform the many fields that depend on such information for routine research as well as advance the development of safe and effective drugs and sustainable food and energy sources.

To meet researchers' needs for both integrative and automated services, the Computational Chemistry Grid (CCG), an NSF project that began in 2004,[1] created the GridChem science gateway (www.gridchem.org). GridChem aims to bring national HPC resources to practicing chemists through intuitively familiar native interfaces. Gateway staff members include chemists, biologists, and chemical physicists who design interfaces and integrate applications, programming experts who layer user-friendly interfaces atop the domain requirements, and HPC experts who coordinate community-wide usage of the integrated services and resources.

System architecture

As Figure 1 shows, GridChem's three-tier architecture consists of a client portal that presents an intuitive interface for data and pre- and postprocessing components, a grid middleware server that coordinates communication between the client and applications via Web services, and applications deployed on the high-performance resources. The software architecture is supported by a consulting portal that addresses user technical issues and an outreach effort that disseminates the gateway's features and responds to the user community's changing needs.

Client portal. The GridChem client is a Java application that users can launch from the GridChem website or download to their local desktop. It serves as the portal to the CCG infrastructure and consists of GUIs for authentication, molecular building, input generation for various applications, job submission and monitoring, and postprocessing. Authentication is hierarchical to serve community users, whose CPU time CCG completely manages, as well as individual users.

The MyProxy repository manages credential delegation. Proxy credentials are used for various services that require authentication. The job submission interface provides multiple ways of generating input files, a resource discovery module with dynamic information, and job requirement definition options. Researchers can use this infrastructure to create multiple independent jobs, and it can launch jobs with diverse requirements simultaneously.

The client also provides a MyCCG module that is central to job-centric monitoring, postprocessing, and potential resubmission mechanisms. MyCCG provides status and usage data for individuals or members of a group under a principal investigator apart from job-specific monitoring.

Middleware services. GridChem middleware services use Globus-based Web services to integrate applications and hardware. Among the services provided are application input specification requirements with default input parameters, queue information, and a simple metascheduling capability based on a "deadline prediction" module supported by the Network Weather Service (http://nws.cs.ucsb.edu/ewiki). The middleware services let MyCCG monitor jobs, provide individual and group usage data, and support dynamic data ingestion with metadata into information repositories.

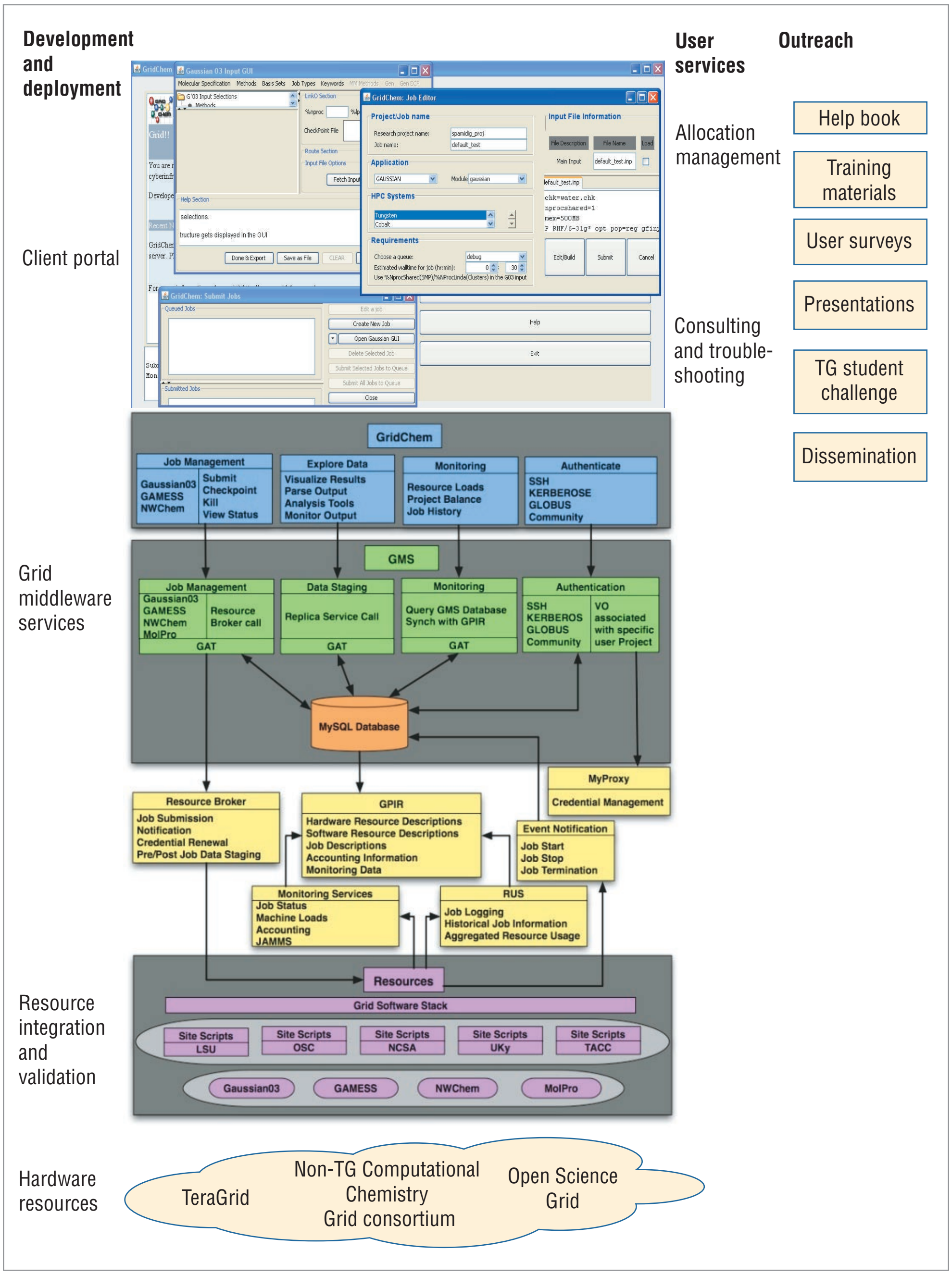

Figure 1. GridChem science gateway. The architecture consists of a client portal, grid middleware services, and deployed applications.

Hardware and application integration. HPC staff deploy and support several popular applications at resource provider sites. GridChem leverages such deployments and abstracts the information needed for their discovery into the Web services database. It tests restart or checkpoint capabilities, where available, and periodically updates software as needed. GridChem controls application access at an individual user level for an individual resource.

GridChem use and future growth

About 300 researchers currently use GridChem, consuming about 80,000 CPU hours per quarter. In the past 18 months, this work has resulted in at least 15 publications in various scientific journals (www.gridchem.org/papers/index.shtml).

As GridChem deploys advanced features such as metascheduling services and integrates material and biological modeling applications, gateway use should grow rapidly in the coming years. The scientific community as a whole will be able to mine the resulting data. The

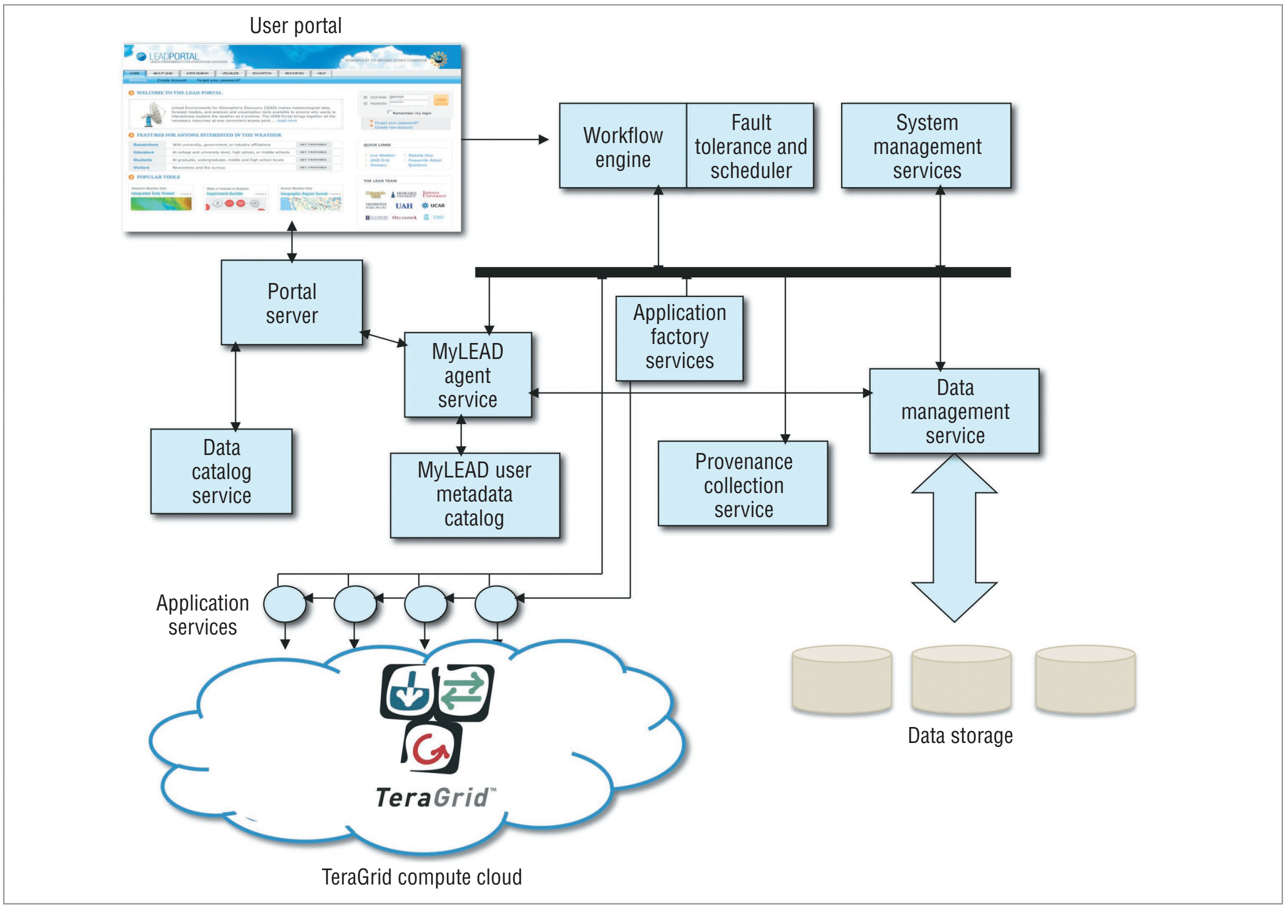

Figure 2. LEAD's Web-service-based cyberinfrastructure. The system has a gateway portal on the front end and uses TeraGrid on the back end for computation, data analysis, and storage.

development of automated metadata collection services for such an information archive will enhance these data mining capabilities.

LEAD

As part of the Large Information Technology Research program, the NSF initiated the Linked Environments for Atmospheric Discovery project in September 2003. LEAD aims to fundamentally change mesoscale meteorology—the study of severe weather events like tornados and hurricanes—from the current practice of static observations and forecasts to a predictive science that responds dynamically and adaptively to rapidly changing weather. Current forecast models are coarse and run on fixed time schedules.

Cyberinfrastructure

One of LEAD's goals is to let any meteorologist capture current weather data and create a specialized high-resolution weather forecast on demand. Another is to assist scientists in using tools that allow the exploration of past weather events and forecasts to create new prediction models. Finally, a major LEAD goal is to find ways in which a weather forecast system can adaptively interact with the measuring instrumentation.[2]

Weather forecasts are complex workflows that filter and normalize data from observational sensors, assimilate it into a coherent set of initial and boundary conditions, and then feed that data to a forecast simulation and finally to various postprocessing steps. In all, a typical forecast workflow might require 7 to 10 data processing or simulation steps, each of which requires moving several gigabytes of data and the execution of a large program.

To accomplish these goals, the LEAD team built a Web-service-based cyberinfrastructure as shown in Figure 2 with a gateway portal on the front end and using TeraGrid on the back end for computation, data analysis, and storage. A set of core persistent Web services communicates both directly and through an event notification bus. Key components include a data subsystem for cataloging experimental results, a workflow execution engine that orchestrates forecast data analysis and simulations, an application factory that manages transient application services that control individual job executions on the back-end TeraGrid computers, and a fault-tolerance and scheduling system to handle failures in workflow execution.

LEAD users

The LEAD gateway is designed to support a wide range of users, from mesoscale meteorology researchers developing new techniques for making accurate on-demand forecasts to high school and college students studying weather modeling and prediction. Both groups have significant requirements that impact the system's design.

Meteorology researchers need the ability to

- configure forecast workflow parameters including the geographic region, the mesh spacing, and various physics parameters and then launch the workflow on demand;
- modify the workflow itself, by replacing a standard data analysis or simulation component with an experimental version, or if necessary create a new workflow from scratch;[3]
- treat each forecast workflow execution as a computational experiment that automatically catalogs metadata, making it possible to later compare all experiments with similar parameter settings or retrieve the complete provenance of every data object; and
- push through a critical forecast of a potentially damaging storm as an "urgent project" by preempting noncritical programs.

In contrast, meteorology and atmospheric science students require

- intuitive and easy-to-use tools for hands-on forecast creation and analysis,
- mechanisms to work in groups and share experiments and data, and
- online education modules that direct the students through different experiments they can do with the tools and data available through the gateway.

Scientists on the LEAD research team principally use the LEAD gateway. Most recently, the gateway played a role in the spring 2008 tornado forecast experiments conducted by the US National Oceanic and Atmospheric Administration's National Center for Environmental Prediction. In 2007, student teams participating in the National Weather Challenge competition also used the LEAD gateway.

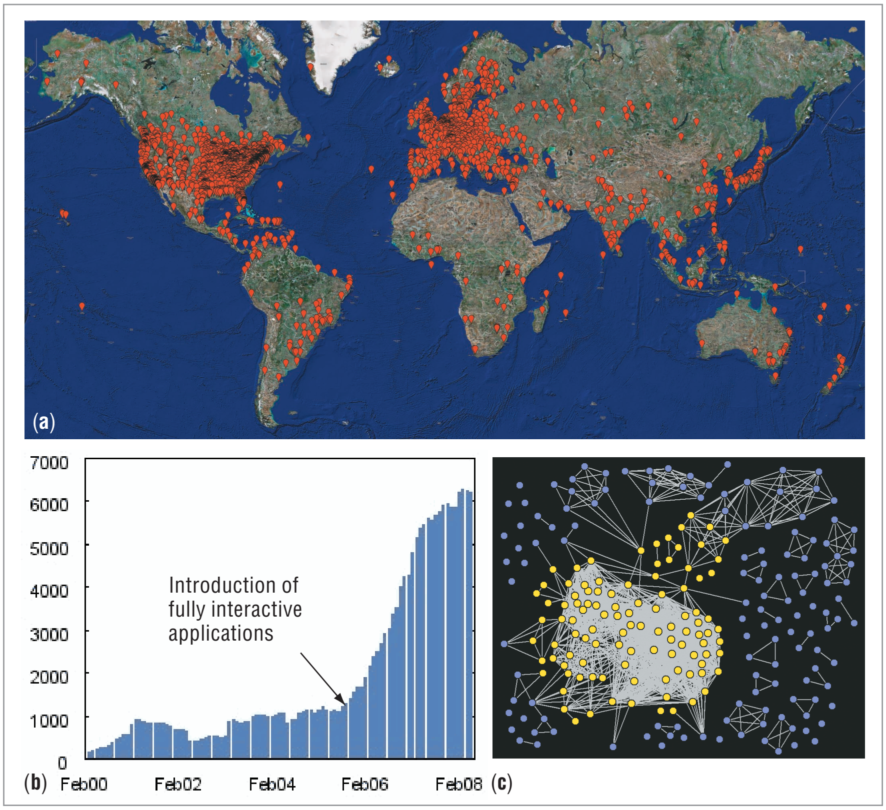

Figure 3. nanoHUB.org usage and impact. (a) The gateway currently serves more than 77,000 users worldwide. (b) Since the introduction of fully interactive applications, the number of annual simulation users has increased sixfold. (c) Social network of 265 nanoHUB citations, with NCN-affiliated authors in yellow (40 percent) and non-NCN-affiliated authors in blue (60 percent); linkages between papers indicate a common author.

nanoHUB.ORG

The NSF-funded Network for Computational Nanotechnology (NCN; www.ncn.purdue.edu) was founded at Purdue University in 2002 to support computational nanotechnology research and education for the National Nanotechnology Initiative. Today NCN operates nanoHUB.org, which, as Figure 3a shows, served more than 77,000 annual users in 172 countries between September 2007 and August 2008; some 6,300 of these users ran more than 340,000 simulations (http://nanoHUB.org/usage).

Interactive simulation and more

The primary nanoHUB target audience is not the small group of nanoscientists with expertise in HPC, grid computing, the message passing interface, scheduling, and visualization but rather the large community of researchers and educators who are primarily nanotechnologists.

Toward that end, all nanoHUB resources are accessible through a Web browser. Users, who might not have

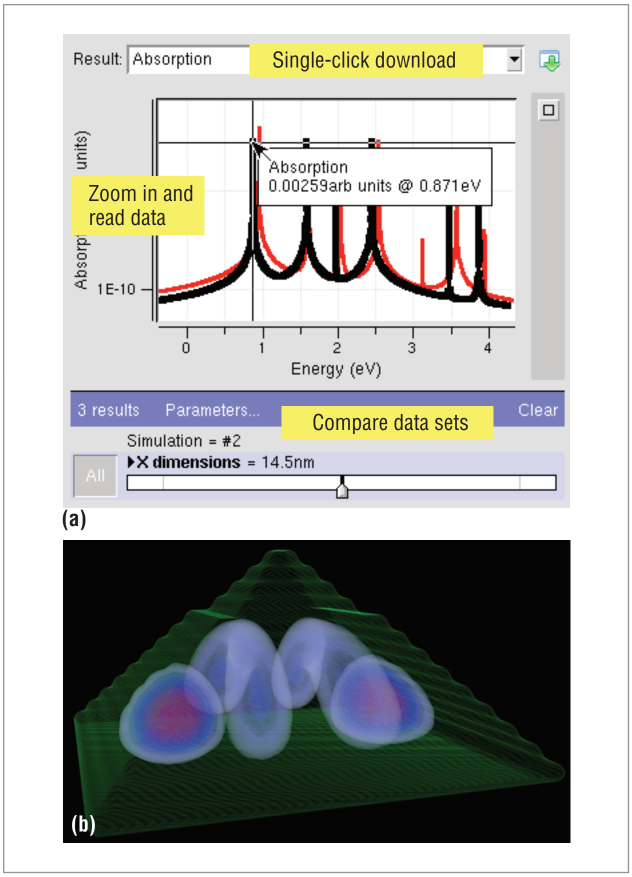

Figure 4. Example screenshots from Quantum Dot Lab simulator. (a) Users can compare datasets from different simulations—in this case, quantum dot size variations. They can zoom in and read data by pointing at it, and download data with a single click. (b) Users can interactively rotate, change isosurfaces, and insert cutplanes using hardware rendered on a remote server. This screenshot shows a volume-rendered 3D wave function of the 10th electron state in a pyramidal quantum dot.

permission to install software, can set up numerical "what if?" experiments and explore data interactively. They can also download and upload data with a simple button click. Figure 4 shows example screenshots from one interactive nanoHUB application, the Quantum Dot Lab simulator (http://nanoHUB.org/tools/qdot).

Online simulation usage data gathered over 12 years shows that the number of nanoHUB tool users is inversely proportional to the tool execution time. Most tools should deliver results in seconds, which implies that they need to be computationally lightweight. Once users are satisfied with general trends in a simulation, they might consider running more detailed models that take tens of minutes, an hour, or all night.

Currently, TeraGrid and the Open Science Grid power six of nanoHUB's 120 tools. With these tools, 145 users ran more than 2,800 jobs that consumed more than 7,500 CPU hours with a total of more than 22,000 hours of wall time during the past year.

In addition to delivering online simulation, nanoHUB supports users with tutorials, research seminars, and a collaboration environment. Researchers can rate and comment on content in a Web 2.0 approach as well as upload content without administrator interference. With more than 1,100 supplemental items, nanoHUB has become a Web publisher.

HUBzero platform

Seven years of experience (1995-2002) delivering online simulations to about 1,000 annual users convinced Purdue researchers that an international cyberresource could make simulation use pervasive and led to the creation of nanoHUB.org. In June 2005, NCN began introducing fully interactive applications, and since then the number of annual simulation users has increased sixfold as shown in Figure 3b. NCN retired Web forms in April 2007.

To accelerate deployment of simulation tools by application developers, including those unfamiliar with Web services, NCN developed HUBzero (http://hubzero.org), a software package that combines the Joomla! open source content management system with two systems developed for nanoHUB applications: the Rappture development environment and Maxwell middleware.

Rappture manages input/output for tools written in C, Fortran, Matlab, Perl, Tcl, Python, or Ruby and various defined workflow combinations without any software rewrites and creates GUIs automatically. Researchers have used Rappture to develop and deploy more than 110 simulation tools in the past three years. While any X11 Unix-based application could be deployed, about 94 percent of nanoHUB applications are Rappture-based, indicating the ease of development in Rappture over other environments. nanoFORGE.org now supports more than 200 application projects using Rappture to Web-enable tools.

Maxwell is a scalable, stable, and testable production-level system that manages the delivery of nanoHUB applications transparently to the end user's browser through virtual machines, virtual clusters, and grid computing environments.

HUBzero is a production-quality platform that has provided better than 99.4 percent uptime to its tens of thousands of users for the past two years.

Researchers outside the nanotechnology realm are using the HUBzero framework, which will be available as open source in 2009, to create gateways to other scientific domains, including cancer care engineering (cceHUB.org), advanced manufacturing techniques (manufacturingHUB.org), global engineering education (GlobalHUB.org), pharmaceutical product development (pharmaHUB.org), and heat transfer (thermalHUB.org). More than a dozen other HUBs are in the pipeline.

Impact on science and education

By cross-fertilizing various nanotechnology subdomains, NCN is extending nanoHUB technology to new communities.[4] As Figure 3c shows, of 265 scientific publications that cited nanoHUB.org and its content, about 60 percent were written by non-NCN-affiliated authors.

An interesting aspect of making simulation tools readily available is that the distinction between research and educational use of nanotechnology resources is diminishing. During the 2007-2008 academic year, for example, more than 40 undergraduate and graduate classes in 18 US institutions used nanoHUB.org tools that previously might have been the province only of researchers. Meanwhile, applications that appear educational to a computational scientist are finding validation in peer-reviewed research.

Designing and constructing a gateway's core software and services requires both cyberinfrastructure specialists and domain scientists.

CABIG

In February 2004, the National Cancer Institute (NCI) launched the cancer Biomedical Informatics Grid (http://cabig.cancer.gov) to speed research discoveries and improve patient outcomes by linking researchers, physicians, and patients throughout the cancer community. Envisioned as a World Wide Web for cancer research, caBIG is a diverse collection of nearly 1,000 individuals and more than 80 organizations including federal health agencies, industry partners, and more than 50 NCI-designated comprehensive cancer centers.

Program goals

Driven by the complexity of cancer and recent advances in biomedical technologies capable of generating a wealth of relevant data, caBIG encourages and facilitates the multi-institutional sharing and integration of diverse datasets, enabled by a grid-based platform of semantically interoperable services, applications, and data sources.[5] The underlying grid infrastructure of caBIG is caGrid,[6] Globus 4-based middleware that implements the required core services, toolkits, and wizards for the development and deployment of community-provided services and programming interfaces for building client applications.

Since its prototype release in late 2004, caGrid has undergone several community-driven evolutions that let researchers without any grid middleware experience rapidly create new services and applications that leverage caBIG's data and metadata.

Challenges

Once the caBIG community had established a foundation for semantic interoperability and developed several data sources, processing vast amounts of data became a priority. While a plethora of software tools and infrastructure exists to address this problem, there are several impediments to leveraging them in the caBIG environment.

First, most caBIG participants do not generally have access to the HPC hardware necessary for compute- or data-intensive analysis. The program's voluntary, community-driven, and federated nature precludes such centralized large-scale resources.

Second, even given access to such resources, most users do not have the experience necessary to leverage the tools commonly associated with access, such as low-level grid programming or executable-oriented batch scheduling. A major emphasis of caBIG is making the grid more accessible, allowing the developer community to focus on creating science-oriented applications aimed at cancer researchers.

Third, services in the caBIG environment present an information-centric view of the data over which they operate. This model provides the foundation for semantic annotations drawn from a shared controlled terminology that, when exposed as grid service metadata, enable the powerful programmatic discovery and inference capabilities that are key to the caGrid approach. This informational model is in stark contrast to the traditional file- and job-oriented views the HPC infrastructure provides.

Science Gateways paradigm

The TeraGrid Science Gateways program provides a convenient paradigm to address these issues. First, it offers an organization and corresponding policies that scientists can use to collectively access TeraGrid's HPC resources rather than having to individually obtain TeraGrid allocations. Second, it abstracts this infrastructure to present unified services to users, most commonly in the form of a Web application or portal.

As caBIG researchers use Web portals or desktop applications that leverage caGrid's various grid services, a science gateway must virtualize access to TeraGrid resources into a caGrid service. In this way, users could be unaware of the underlying implementation's use of TeraGrid, much as other science gateway users might be unaware of TeraGrid accounts, allocations, or resource-providing service interfaces such as the GRAM service.

Implementations

The initial gateway grid service implementation performed hierarchical cluster analysis of genomic data,[7] an analysis routine available to the caBIG community with only modest computational needs. The caBIG team successfully demonstrated the utility of the gateway approach by utilizing this service in the existing geWorkbench desktop application to perform an analysis and visualize the results. Beyond the actual software, they created a set of best practices and guidance documents to better inform future efforts.

The prototype caGrid science gateway service was well received by the caBIG community and set the groundwork for numerous additional gateway services for other problem domains. More tools are needed to further simplify the process, but providing caBIG application developers a common environment of strongly typed, semantically described grid services that harness TeraGrid's computing power is a worthwhile investment given the large quantities of data and analysis routines expected to be developed in caBIG.

The first phase of the TeraGrid Science Gateways program has yielded several lessons.

First, developing a gateway from scratch can require substantial effort. Designing and constructing the core software and services requires both cyberinfrastructure specialists and domain scientists. Consequently, the program has focused on gathering and deploying building blocks such as portal frameworks, security tools (certificate repositories and auditing tools), common services, reusable workflow engines, application wrapping and deployment tools, and directory services. A reasonable goal, almost within reach, is to provide any team of dedicated domain experts with a toolkit, training documentation, and technical assistance that would let them build and populate a gateway in a week.

Traditionally, computational scientists have been patient and persistent, willing to deal with complex hardware and software systems with high failure rates. Because supercomputers still use batch queues, users must sometimes wait for hours without any intermediate feedback to see if the latest changes to a runtime script will result in a successful execution. On the other hand, science gateway users expect nothing less than the same ease of use, on-demand service, and reliability that they have grown to expect from commercial portals that cater to online financial transactions or information retrieval. The key emphasis must therefore be on usability. User-friendly and stable gateways could open HPC modeling capabilities to a broad user base that Unix-based TeraGrid access never would have reached.

In addition, TeraGrid has had to devote a substantial effort to making its grid infrastructure more reliable and scalable. This has been especially challenging because a grid of supercomputers is not the same as a commercial data center that has been designed from the ground up to support very large numbers of interactive remote users.

Often, the greatest benefit to users is easy access to data and the tools that can search, filter, and mine it. To have a truly significant impact, the gateway must provide more capability than a desktop machine yet be as easy to operate as any desktop software without any grid or HPC-specific knowledge. We anticipate that future gateways will integrate with social networking technologies that can aid students and enable a community of scientists to share tools and ideas.

Gateway usage can be relatively easily monitored in terms of number of users, simulation runs, CPU times consumed, and so on. However, a gateway's scientific and educational benefits are more accurately measured by classroom usage, citations in the literature, and user case studies—metrics that are more difficult to gather.

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