



THE ORGANIZATION AND MANAGEMENT OF GRID INFRASTRUCTURES

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Grid computing technology has become fundamental to e-Science. As the virtual organizations established by scientific communities progress from testing their applications to more routine usage, maintaining reliable and adaptive grid infrastructures becomes increasingly important.

For nearly a decade, high-energy physics (HEP) has been a driving force behind the development of grid computing technology and e-Science infrastructures worldwide. A grid is a service for sharing computer power and data storage capacity over the Internet. It goes well beyond simple communication between computers, ultimately aiming to turn the global network of computers into one vast resource for solving large-scale compute- and data-intensive applications.

A computational grid is often compared to an electric power grid in which the power generators are distributed and users can access power without regard for the

source of energy and its location. A key element of grid computing is that it enables collaboration between geographically dispersed communities in the form of virtual organizations.

This new, powerful technology has greatly impacted modern science.^{1,2} Although HEP remains the largest and most demanding community, production-quality grid infrastructures have emerged in Europe and the US that sustain high daily workloads and support many types of e-Science.

LHC COMPUTING GRID

In the late 1990s, physicists designing computing models for experiments using the Large Hadron Collider, a next-generation particle accelerator at CERN in Geneva, Switzerland, due to come online in 2009, were faced with the problem of using widely dispersed resources to obtain the total computing and storage capacities required. To address this challenge, detailed in the "LHC Experiments" sidebar, they proposed a hierarchical model based on a tiered structure of regional computing centers (<http://cern.ch/MONARC>). At the same time, the Globus Project was demonstrating grid technology developments.

→ LHC EXPERIMENTS

The Large Hadron Collider (<http://lhc.web.cern.ch/lhc>) is the world's largest and most powerful particle accelerator. It consists of a ring of superconducting magnets 27 kilometers in circumference that accelerates opposing beams of protons or lead ions and collides them head-on at very high energy in the center of four large detectors. LHC will accelerate the proton beams to 7 teraelectron volts each, representing a sevenfold increase in energy over existing accelerators. In addition, the intensity of the beams in the LHC will be many times more than that in previous accelerators.

These factors mean that the collision rates are several orders of magnitude greater, and that the prospects for discovering new physics that transcend the so-called "standard model" are unprecedented. The standard model has been very successful in explaining the fundamental interactions of elementary particles but does not give the full picture. In particular, it does not account for the origin of mass, and this is one of LHC's primary goals.

The accelerator and four large experiments are situated 100 meters underground. Two of the experiments, ATLAS (A Toroidal

LHC Apparatus) and CMS (Compact Muon Solenoid), are huge general-purpose detectors that together aim to discover the Higgs boson and the dimensions of dark matter. Two other large detectors have more specific tasks: ALICE (A Large Ion Collider Experiment) will study lead ion collisions to understand the quark-gluon plasma, a state of matter believed to have existed just after the Big Bang, while LHCb (Large Hadron Collider beauty) will explore why our universe is made almost entirely of matter and almost no antimatter.

Each detector has around 100 million individual electronic sensors that read out each time there is a collision—some 40 million times a second. LHC uses sophisticated hardware and software processors to filter the resulting avalanche of data to select potentially interesting events. The result of this filtering is a data stream of 200-300 megabytes per second from each of the two largest detectors that must be archived on tape and later analyzed. In total, the four experiments will produce some 650 MBps of data—about 1 CD's worth every second. ALICE alone will produce some 1.25 GBps of data to be processed during the time the accelerator runs with lead ions.

The match between HEP needs and this new technology became apparent at the International Conference on Computing in High Energy and Nuclear Physics in 2000, and a series of projects in the US and Europe to build prototype "data grids" to understand the technology and its application to HEP problems rapidly followed. An early example of this was the EU-funded DataGrid project (<http://eu-datagrid.org>), which ran from 2000 to 2004 and established a testbed for HEP, life science, and earth science applications.

CERN scientists initiated the LHC Computing Grid (LCG) project to create a computing environment that would meet the LHC experiments' unprecedented storage and computing needs. It is estimated that these experiments will generate some 15 petabytes per year of data—equivalent to about 3 million DVDs—that must be stored and distributed to thousands of scientists in hundreds of laboratories across the world, while around 100,000 processors will be needed in the first years to process and analyze the data.

While the scale of data processing made grid technology a natural choice for the LHC experiments, locating sufficient computing resources at CERN is also limited by practical considerations. Realistically, it is more straightforward to request funds for computing and storage installed in universities and at national labs than to send them to CERN. Thus, the LHC computing environment had to be distributed to use the available resources.

LCG began with the goal of integrating grid technology that had been prototyped and demonstrated in testbed environments with the existing production computing environments of typical HEP computer centers. In its first two years, LCG built a grid of around 40 sites that the

experiments started to use for simulation work as well as for learning how to build applications on top of the grid services.

WORLDWIDE LCG

The LCG evolved into the Worldwide LHC Computing Grid (<http://lhc.web.cern.ch/LCG>), a collaboration that now includes some 150 sites in 35 countries.

The computer centers that participate in WLCG are party to a memorandum of understanding (MoU) that defines the levels of resources to be provided, as well as services and service levels. The centers rely on various grid infrastructure projects—primarily Enabling Grids for E-science (EGEE; www.eu-egee.org) in Europe and the Open Science Grid (OSG; www.opensciencegrid.org) in the US—to provide the tools, services, and support structures needed to fulfill the MoU's requirements. Through the grid infrastructures, members of the global physics community will work together to analyze this data, which it is hoped will lead to discovery of the Higgs boson, an important step in the confirmation of the "standard model" in particle physics.

A key metric for WLCG is the ability to push data out of CERN to 11 regional (tier 1) computer centers, which provide data analysis facilities and in turn send processed data to the smaller (tier 2) centers where physicists analyze it. The aggregate data rate from CERN to the tier 1 centers must exceed 1.3 gigabytes per second to keep up with the data-taking rate. Figure 1 shows the achieved rates during one four-day test and clearly demonstrates that WLCG easily reaches the required rate and comes close to 3 GBps for extended periods. This margin provides the ability to "catch up" if one of the tier 1 centers is temporarily unavailable.

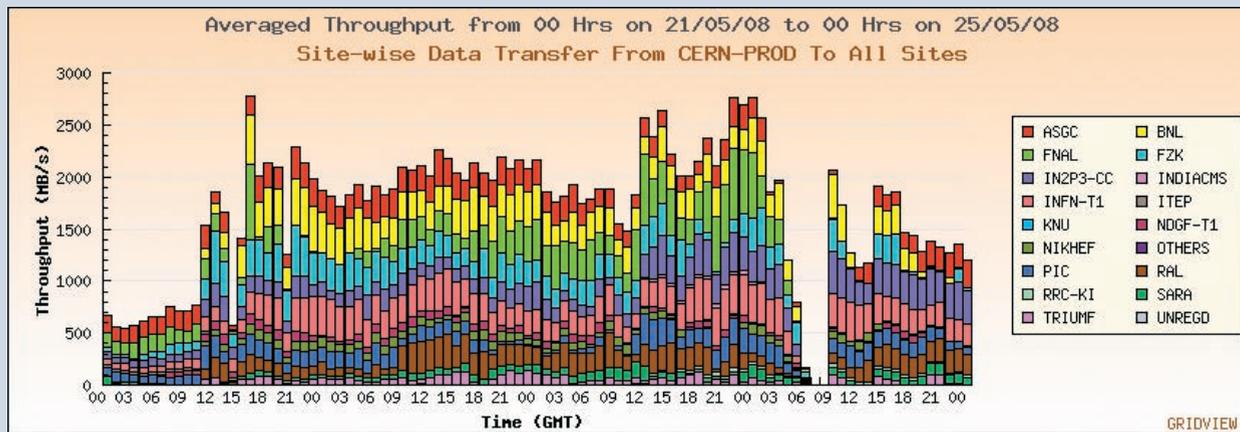


Figure 1. Average throughput for HEP experiments, 21-25 May 2008. WLCG easily achieves the required aggregate data rate of 1.3 gigabytes per second and for extended periods comes close to 3 GBps.

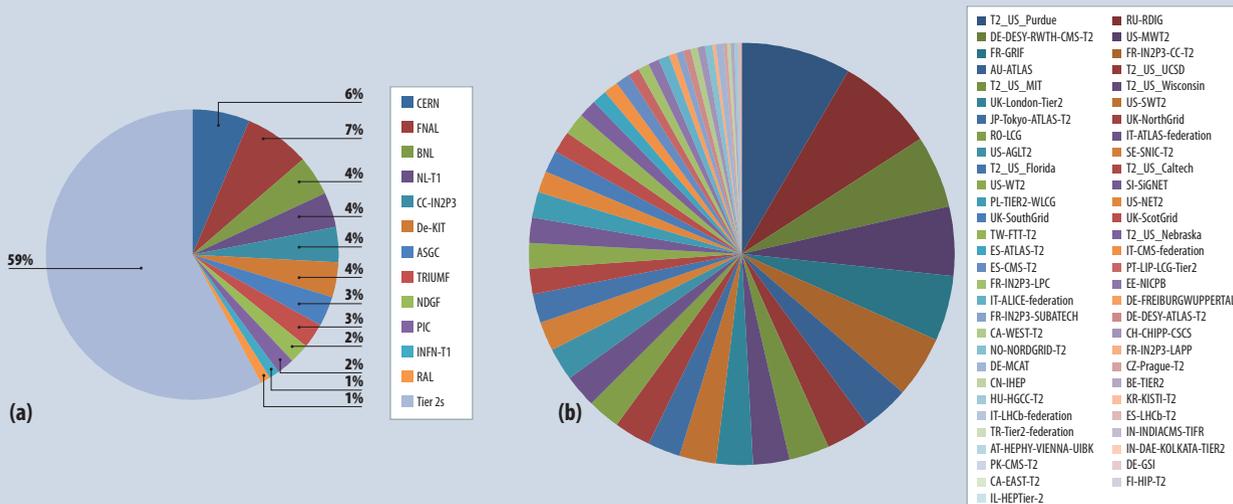


Figure 2. Workload distribution at WLCG centers. (a) Distribution of work among CERN and the tier 1 and tier 2 centers. (b) Breakdown of work among tier 2 "federations"—management groupings of sites.

Data transfers between all tier centers for one test achieved aggregate rates of up to 200 terabytes per day. These transfers use tools built on top of the GridFTP protocol to provide reliability and error recovery. When LHC is fully operational, data from the experiments will account for more than 60 percent of the load on the EGEE grid infrastructure.

Looking at the amount of work performed across the range of sites that participate in WLCG, it is clear that all of them contribute to the overall computing load. Indeed, as Figure 2 shows, the tier 2 sites consistently provide more than half of the total CPU cycles delivered to WLCG, with contributions at all scales. This means that all LHC collaborating institutions can contribute, and more importantly

that the experiments can use these resources. This accomplishment vindicates the grid computing approach and justifies the hard work invested by CERN over the past five years.

Since 2004, WLCG has been running a series of increasingly demanding tests on the system in preparation for the LHC start-up. These tests have been a key to driving improvements in functionality, reliability, and service levels. Notable among these tests are the Service Challenges, which go beyond simply testing grid throughput to stressing the end-to-end service, separating this from potential problems with the applications. These challenges involve participation by all members of the WLCG collaboration, including EGEE sites and other sites in Asia and the US.

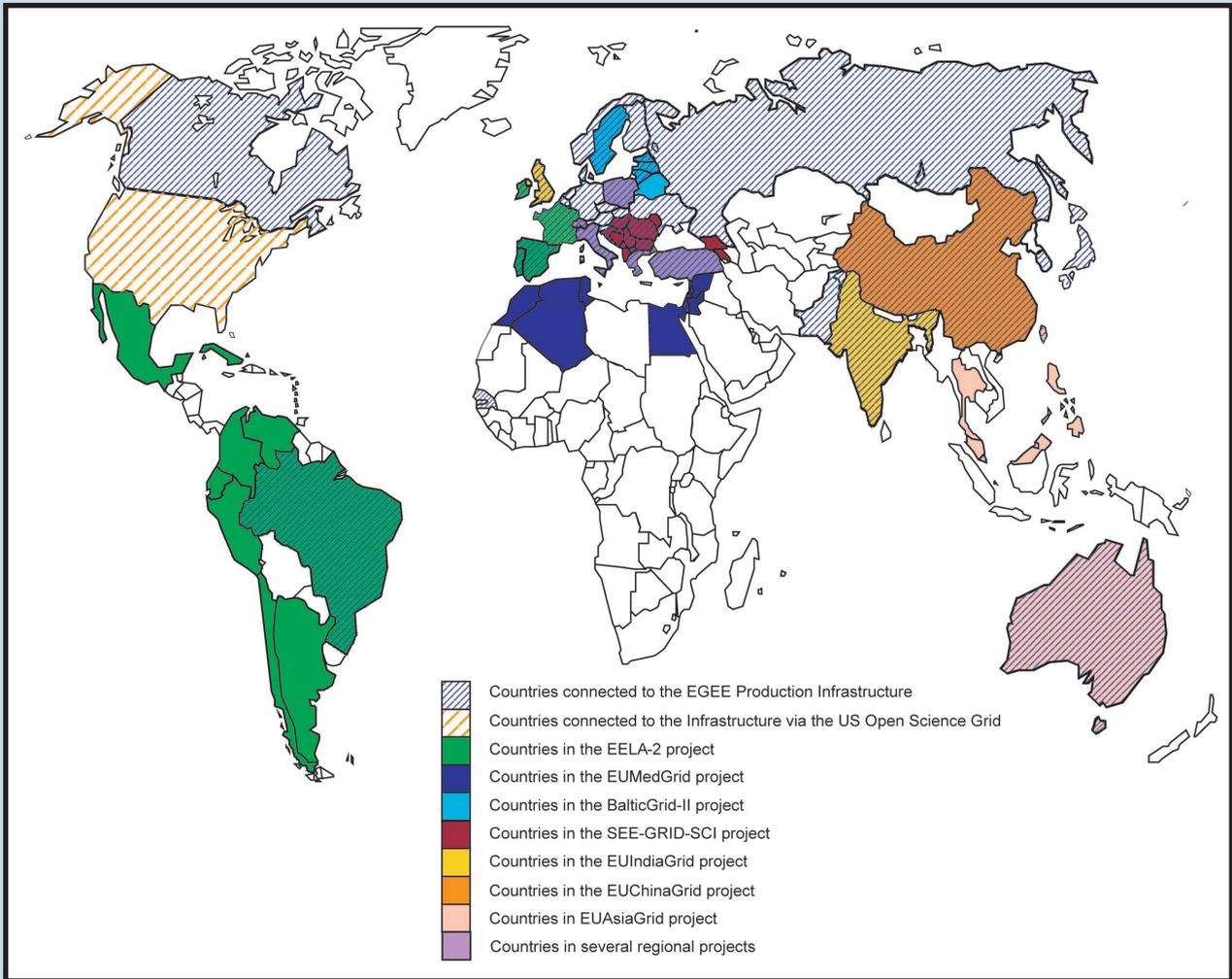


Figure 3. Countries within EGEE or connected to its multidisciplinary grid infrastructure via collaborative projects.

The most recent testing occurred in May 2008 and was designed as a final demonstration of the system's readiness, with all experiments running their full computing chains from data acquisition to analysis. WLCG showed the ability to support workloads well in excess of 500,000 jobs per day across the participating grid sites. This workload and the data transfer metrics, as well as the sustainability of running the service at these levels, suggest that WLCG will be capable of meeting the LHC needs at the scale required. To date no other application community has expressed such large-scale needs.

ENABLING GRIDS FOR E-SCIENCE

WLCG relies on EGEE as the provider of the underlying grid infrastructure in Europe, enabling it to focus on higher-level services and quality-of-service issues that are important to the HEP community. Since EGEE assumed management and operation of the grid infrastructure in

2004, it has expanded to support about 250 sites in more than 40 countries, with corresponding increases in the resources available through the infrastructure.

World's largest grid infrastructure

EGEE serves a wide range of European scientific communities and is currently the largest, most widely used multidisciplinary grid infrastructure in the world. Figure 3 illustrates how global collaborations have extended EGEE's reach to benefit European science.

Built on the pan-European GÉANT2 network (www.geant2.net), EGEE gives researchers 24/7 access to computing, storage, instrumentation, and informational resources and enables them to easily work together on common challenges. New collaborations and services continuously arise, and EGEE adapts to accommodate them. Strong quality-assurance, training, and outreach programs contribute to the infrastructure's success.

➔ A VISION FOR CYBERINFRASTRUCTURE

Edward Seidel, José L. Muñoz, Steve Meacham,
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What are the three-dimensional structures of all of the proteins encoded by an organism's genome, and how does its structure influence function? What patterns of emergent behavior occur in models of very large societies? What are the mysterious gamma-ray bursts that are observed throughout the distant reaches of the universe? What abrupt transitions can occur in Earth's climate and ecosystem?

Answering these kinds of complex questions often requires a comprehensive approach that integrates theory, experiment, observation, computer simulation, and data analysis. Increasingly, such problems depend critically on advances in cyberinfrastructure.

The National Science Foundation created the Office of Cyberinfrastructure (www.nsf.gov/dir/index.jsp?org=OCI) in 2006 to address the high-performance computing (HPC) needs of the US scientific community, although its roots go back more than two decades. NSF's broad mission covers all of the basic sciences—including physics, astronomy and astrophysics, chemistry, biology, geosciences, and mathematics—as well as social and behavioral science and economics. To advance the sciences, OCI in recent years has been building on the foundation of the national supercomputing centers program started in the 1980s, and the TeraGrid that began in 2001, to greatly expand the availability of HPC facilities and integrated digital services to academic researchers.

The OCI Track 2 program has made a series of new investments in supercomputing facilities that will increase the TeraGrid's entire computing capacity by an order of magnitude, while the Track 1 program will deliver a single sustained petascale computing facility at the University of Illinois called Blue Waters (www.ncsa.uiuc.edu/BlueWaters) that will routinely deliver multiple petaflops on real applications. Blue Waters researchers will be able to attack the most challenging science and engineering problems, such as understanding gamma-ray bursts, high-resolution climate forecasting, and designing new materials atom by atom.

Along with the US Department of Energy, NSF also supports the Open Science Grid, a collection of university resources that in aggregate provide access to roughly 50,000 compute cores across dozens of campuses for data- and compute-intensive jobs serving the high-energy physics, gravitational astronomy, and other science communities in the US and abroad.

OCI is enhancing these programs with a new generation of high-end data and digital services motivated by the need to study complex problems that require a more comprehensive cyberinfrastructure.

Science activities in every domain, whether experimental, theoretical, or computationally oriented, are becoming increasingly data-driven, and the extensive amount of information generated by research communities, observation systems, experiments, sensors, and supercomputers is rapidly overwhelming our ability to handle it. For example, the National Ecological Observatory Network (www.neoninc.org) will soon produce 150 terabytes of data per year, the Large Synoptic Survey Telescope (www.lsst.org/lstt) will generate 30 terabytes of data in a night, and a single gamma-ray burst simulation on Blue Waters could yield 5 petabytes of data in a few days.

OCI's initial efforts to address this new world include Sustainable Digital Data Preservation and Access Network Partners (DataNet) and eXtreme Digital Resources for Science and Engineering (XD). DataNet aims to build a network of high-end data

nodes providing data collection, mining, and curation services for multiple communities. XD seeks to provide high-end digital services to the nation's academic community, integrating national supercomputing and data centers with one another and the campus-based researchers they serve.

To handle these extraordinary requirements, network technologies are rapidly advancing, with optical networks routinely providing 10 gigabits per lambda, with 100-Gbit and even terabit networking just around the corner. NSF is responding by providing global network connections through its International Research Network Connections (IRNC) program, and by working with various partners in the US, including regional optical network organizations, to provide connectivity across the nation. Programs like these will need to be expanded to meet future data growth.

Cyberinfrastructure technologies are on exponential growth paths, and the complexity of these systems and the corresponding difficulty using them are likewise increasing exponentially. As researchers begin to address more real-world science and engineering challenges, the distinction between theoretical, experimental, observational, and simulation-based approaches will blur—all approaches will be needed to solve any one of these problems.

More advanced tools will thus be required to close the gap between the advanced cyberinfrastructure being deployed and our ability to effectively exploit it. However, it is often said that the current "software crisis" will only worsen as the systems we deploy become increasingly complex and are needed in multi-tiered combinations. For example, consider the many problems posed by a hurricane approaching a coastal population center. Where will the hurricane go? What will the resulting storm surge bring? Where should supplies be sent? What transportation patterns should be followed? How should officials and the public respond? Responding to this single weather event requires a combination of observation, coupled simulations, and software that goes far beyond using large-scale supercomputers and grids.

Perhaps the greatest scientific challenge is developing the training and expertise needed to use advanced cyberinfrastructure to solve complex problems. This requires understanding the social as well as the technical challenges of distributed collaborations and virtual organizations.

NSF will continue to expand its mission to provide the necessary cyberinfrastructure, including hardware, software, computational science activities, and, most importantly, development of human capital needed to address these challenges in the 21st century.

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To achieve its ambitious goals, EGEE has continuously nurtured strong links to other major grid projects around the world including the OSG and TeraGrid (www.teragrid.org) in the US, the Japanese National Research Grid Initiative (NAREGI; www.naregi.org) and the Distributed European Infrastructure for Supercomputing Applications (DEISA; www.deisa.org), some of which have common partners with EGEE. Shared work with these projects includes the areas of grid security, infrastructure, interoperability, and user community support. In addition, EGEE collaborates with numerous grid projects that extend the infrastructure to new geographical areas or application domains.

Work is also under way to help expand the adoption of EGEE's gLite (www.glite.org), an open source middleware distribution that combines components developed in various related projects—in particular Condor and Globus—via the Virtual Data Toolkit, and to provide support in areas such as grid training, dissemination, and security.

Large-scale, data-intensive, distributed computing

EGEE has proven the viability of a computing grid infrastructure that meets the large-scale, data-intensive, and distributed computing requirements of e-Science. The EGEE production service currently has access to more than 20 petabytes of storage and 80,000 CPUs, with these numbers expected to rise dramatically during the next year as extra resources for the LHC experiments and other new applications come online. Already these figures considerably exceed the project's initial goals, demonstrating the enthusiasm within the scientific community for EGEE in particular and grid solutions generally.

In 2006, the EGEE production service processed 19.6 million jobs (a job is a run of a single program to process data that lasts about 8-12 hours) totaling 8,400 CPU-years. The following year this figure rose dramatically to 44 million jobs, and it continues to increase. At least 100 different applications today regularly use the EGEE infrastructure, with more than 10,000 scientists benefiting from the results of this distributed computation.

VIRTUAL ORGANIZATIONS

The concept of the virtual organization is a fundamental part of the security model of a large production grid infrastructure such as EGEE. Researchers form VOs to collaborate, share resources, and access common datasets via the grid infrastructure. The original idea of a VO as a dynamic group of users with a common goal coming together for a specific, short-lived collaborative venture and then dissolving has never been realized owing to the complexity of deploying and authorizing such a dynamic structure.

The VO is a basic building block of a grid. The typical VO tends to be a relatively long-lived organization that

brings together a group of researchers with a common purpose. Some VOs can be very large—for example, each LHC experiment is managed by a single VO that might have upward of 2,000 members. On the other hand, there are application domains such as biomedicine where a single VO can contain several subgroups that agree to collaborate on specific topics but actually have little interaction with one another.

EGEE already supports more than 200 VOs. These include groups actively supported by EGEE, with help being provided for application porting and the inclusion of special features into gLite, and groups that simply use the general services EGEE provides. So far, no other active VOs have such demanding data-management requirements. Indeed, it is the complexity and scale of the data-management needs that distinguish the LHC experiments, which depend completely on grid infrastructures to provide the necessary computing resources.



The concept of the virtual organization is a fundamental part of the security model of a large production grid infrastructure such as EGEE.

VO CHARACTERISTICS

Sometimes e-Science projects fail not because of the technologies but because of problems associated with organizing and managing grid infrastructures through VOs. Three useful definitions help clarify why VOs can be difficult to manage.

A decade ago, organizational theorists Gerardine De-Sanctis and Peter Monge defined a VO as “a collection of geographically distributed, functionally and/or culturally diverse entities that are linked by electronic forms of communication and rely on lateral, dynamic relationships for coordination.”³ This definition emphasizes distribution, diversity (functional and cultural), and coordination (lateral communication and dynamic relationships).

A few years later, Ian Foster, Carl Kesselman, and Steven Tuecke defined a VO as “flexible, secure, coordinated resource sharing among dynamic collections of individuals, institutions, and resources.”⁴ According to this definition, a VO's characteristics include flexibility, security, coordination, and dynamics (which can be subsumed under coordination).

In June 2008, the US National Science Foundation's Office of Cyberinfrastructure solicited a study on VOs as sociotechnical systems.⁵ According to the solicitation,

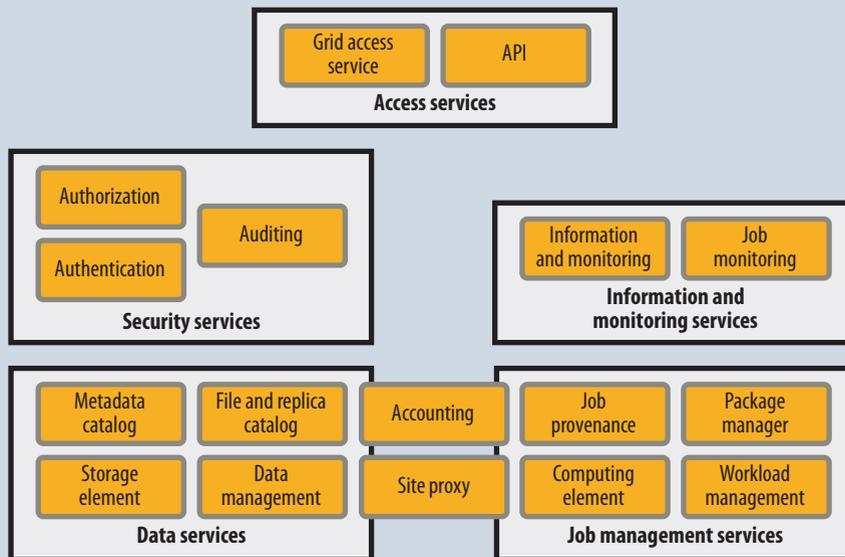


Figure 4. EGEE gLite components. The middleware provides users with high-level services for scheduling and running computational jobs, accessing and moving data, and obtaining information on the grid infrastructure as well as grid applications, all embedded in a consistent security framework.

“a virtual organization is a group of individuals whose members and resources may be dispersed geographically, yet who function as a coherent unit through the use of cyberinfrastructure.” This third definition highlights dispersion—the same thing as distribution in the first definition—and coherence (functional) as two additional characteristics of a VO.

Taking these definitions together, a VO can be characterized by *dispersion/distribution*, *diversity*, *coherence*, *security*, *coordination*, and *flexibility*. Such an organization is highly complex, particularly when enabled by large-scale, data-intensive, and distributed infrastructures such as those in e-Science.

Complexity theory is a useful framework for examining the relationship between VOs and technologies. In the theory’s social-scientific version, individuals and groups are the basic elements and three interrelated principles guide VO management: *nonlinearity*—dispersion of management, support, and diversity among service groups, countries, and disciplines; *emergence*—coherence through standards, interoperability, and security by policies and middleware; and *self-organization*—coordination by grid management oversight, automation, and service-level agreements (SLAs), and flexibility by middleware and scalability.

Nonlinearity

Nonlinearity is said to exist when a system is not in equilibrium or “far-from-equilibrium.”⁶ This is a state for all living systems and organizations. Nonlinearity contributes to a system’s transformation and evolution. In a VO,

geographical dispersion/distribution as well as functional and cultural diversity add to its nonlinearity.

Dispersion/distribution. The computing and storage resources integrated in EGEE are provided by a large and growing number of resource centers, mostly in Europe but also in the Americas and Asia, coordinated by regional operations centers (ROCs).

EGEE’s distributed operation model is a key to the project’s success—a centralized operational model would not be scalable to the large number of federated sites. The infrastructure’s scale and workload continue to increase in terms of sites and CPUs without any impact on its overall operations.

The EGEE production infrastructure also provides a fully distributed support network for operations and traditional user support. It is novel in bringing together individual local support structures as well as providing a central coordination point. The same is true of the operational security activities—EGEE provides a layer of coordination and addresses grid issues in supplementing local security efforts.

Diversity. Functional diversity is inherent in EGEE’s middleware distribution. The focus of gLite is on foundation services that provide the basic middleware infrastructure that defines the EGEE grid. It also provides users with high-level services for scheduling and running computational jobs, accessing and moving data, and obtaining information on the grid infrastructure as well as grid applications, all embedded in a consistent security framework. Figure 4 gives an overview of the gLite services.

→ e-INFRASTRUCTURES: CATALYSTS OF A NEW SCIENTIFIC RENAISSANCE

Mário Campolargo, *European Commission*

We face an epochal change in the way of doing science. Enabled by high-speed research networks, increasingly powerful computers, grid technologies, data infrastructures, and global virtual collaborations, e-Science is accelerating the pace of discovery and innovation and providing scientists with more efficient and cost-effective ways to respond to future societal expectations.

To support the move toward e-Science, the European Commission has made significant investments in e-infrastructures within the context of the EU multiannual Framework Programmes for Research and Technology Development.

An *e-infrastructure* is an environment where resources—hardware, software, and content—are readily accessible and can be easily shared. It integrates networks, grids, middleware, computational resources, experimental workbenches, data repositories, tools and instruments, and operational support for virtual organizations.

Five e-infrastructure domains together provide a variety of functions and services that underlay the scientific discovery process (<https://cordis.europa.eu/fp7/ict/e-infrastructure/home-en.html>):

- research networks such as GÉANT2, the world's largest multigigabit communication network dedicated to research and education, connecting around 4,000 universities and research centers and similar networks worldwide;
- grid infrastructures such as Enabling Grids for E-science (EGEE) and Distributed European Infrastructure for Supercomputing Applications (DEISA) that support the demands of high-energy physics, bioinformatics, and other disciplines to share and federate the power of computers and sophisticated, often unique, scientific instruments;
- data repositories and related tools and methods to ensure the availability, treatment, and preservation of scientific content resources including reports, articles, experimental and observational data, and rich media;
- supercomputing projects such as Partnership for Advanced Computing in Europe (PRACE) that aim to establish a petascale supercomputing ecosystem and related modeling and simulation environments; and
- global virtual research communities—rich sets of tools empowering complementary scientific organizations to use e-infrastructures and set up virtual collaborations to address research challenges of global relevance.

Over the years, the development of e-infrastructures has been driven by a twofold strategy of providing high-quality produc-

tion-level services to scientists while encouraging, whenever possible, the use of leading-edge technologies and solutions to allow precommercial testing and experimentation.

For example, GÉANT2 provides top-of-the-range network connectivity performance aiming at exascale dimensions by 2020. The Federated e-Infrastructure Dedicated to European Researchers Innovating in Computing Network Architectures (FEDERICA) project (www.fp7-federica.eu) seeks to virtualize GÉANT2's routers to enable the coexistence of several networks on the same infrastructure to test new architectures and protocols for the future Internet.

The use of Web 2.0 technology to enhance creativity and information sharing in research has opened new opportunities for cross-border multidisciplinary collaborations. Designed to support these "participative" paradigms, e-infrastructures facilitate the emergence of global virtual research communities, which mark a cultural shift in the way scientific knowledge is produced, disseminated, and injected in innovation life cycles.

The involvement of industry in the development of e-infrastructures is also critical. Research and development in supercomputing technologies, for example, has considerably impacted the competitiveness of an entire ICT ecosystem encompassing computer manufacturers, software and services providers, system integrators, and industrial users.

With more than \$600 million planned to be invested in the period 2007-2013, Europe's response to the long-term challenges of e-Science is strong and determined. However, to fully exploit the potential of global scientific collaboration, the research community must overcome numerous obstacles. These relate in particular to the clash of cultures among different disciplines, the need to rethink organizational models, and the establishment of quality assurance mechanisms and business models.

New strategies for technological development of e-infrastructures are therefore fundamental to ensuring "future-proof" solutions based on open standards that can be maintained and improved in the long run and add value to research and innovation investments. With such strategies in place, e-infrastructures can be the catalysts of a new scientific renaissance that will pave the way for a new industrial and societal revolution.

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Cultural diversity is apparent in EGEE's distribution among numerous countries, but there is also a high degree of disciplinary diversity. While the needs of HEP, especially the LHC experiments, continue to be the main impetus behind grid technology development, non-HEP applications are responsible for around one-third of EGEE's total workload, and the percentage is increasing.

A growing number of application domains are using EGEE. These include astrophysics, computational chemistry, earth and life sciences, finance, fusion science, and

geophysics, with many others currently evaluating the infrastructure. EGEE also works with business users and industrial service providers to ensure technology transfer to various business sectors.

Along with the dispersion of management and support, the wide range of diverse service groups, countries involved, and disciplinary domains keep EGEE and its VOs in a far-from-equilibrium state of nonlinearity. Whenever a new piece of technology is added to a system, it drastically changes the behavior of the entire organization and

produces unpredictable results.⁶ The same is true when EGEE adds a new service, country, or discipline.

Emergence

In complexity theory, emergence refers to “something that is genuinely new, not simply perceived as new.”⁶ A phenomenon can emerge simply because the conditions for it are present. One important effect of production grid infrastructures has been the triggering of new collaborations and research possibilities that were not otherwise possible.

A good example of this is Wide In Silico Docking on Malaria (<http://wisdom.eu-egee.fr>), an initiative for grid-enabled drug discovery against neglected and emergent diseases. In one test, WISDOM collaborators evaluated almost 200 million possible arrangements between drug components and target proteins of the malaria parasite in a few weeks—the equivalent of hundreds of years of a single



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PC's computing power. Another test analyzed 300,000 drug potential components for the potentially lethal H5N1 avian influenza virus.

A property can also emerge out of individual actions in response to the external environment. Functional coherence and security are two emergent properties in a VO, which aim to coordinate people and resources toward a common goal. Without these properties, a VO cannot support e-Science projects.

Coherence. Functional coherence refers mainly to standards and interoperability. Most European countries have grid infrastructures, at varying levels of maturity, yet a limitation of national grids is their inaccessibility to international scientific communities. Beyond the national level, standards become important to allow ease of connectivity and sharing of applications. EGEE ensures that Europe's grid infrastructure does not fragment into national and thematic grid infrastructures, with less coherence at a European level.

EGEE plays an active role in standards setting and is involved in global standards bodies such as the Open Grid Forum (OGF; www.ogf.org). This participation enables the project to pursue the goal of producing middleware components that are, from their conception, interoperable with those coming from other providers.

It is vital that EGEE works to ensure continued interoperability of its infrastructure with other international grids. EGEE also must be able to coexist with local/campus, regional, and national grids on the same hardware. The closer together these infrastructures can be, the more likely a site will be integrated into EGEE.

The OSG has achieved full production-level interoperability, and other infrastructures are making good progress. However, EGEE has taken a conservative approach in defining the gLite composition, avoiding frequently changing software while tracking emerging standards.

In the first phases of the project, EGEE researchers developed a good set of tools that they will revise and coordinate at the level of information gathering and publishing. The researchers will further enhance standard formats and interfaces, already proposed as prototypes, to permit data gathered by various tools to be presented to service managers coherently and consistently. Such standards will increase the scope for sharing tools and monitors and avoid duplication of development and monitoring.

An important adjunct to the tools themselves will be the continued and evolving use of SLAs to set standards for site and service levels. This mechanism and the reporting and publication of the associated metrics will exert pressure to provide reliable and effective services, which will also help reduce the level of required grid oversight.

Research does not stop at national borders, and, while national infrastructures are fundamental in providing local connectivity and resources to researchers, they must be linked seamlessly with other grids around the world to enable global scientific collaboration. With the support of EGEE and the European Commission, many European countries have established national grid initiatives. Currently at different levels of maturity and implementation, these initiatives ultimately aim to provide a common infrastructure in support of all e-Sciences.

Security. The EGEE production service has access to a large amount of computing power and storage, which will continue to increase as additional resources for the LHC experiments and other new applications come online. Due to the scale of data and resources involved, security is a high priority for VOs in e-Science.

Policies facilitate security in a VO and are vital to enabling a true production service rather than extended testbeds. EGEE has a broad range of policies that address important operational and security concerns. The intent is not to replace local policies but to supplement them and provide the overall framework. EGEE's policies have evolved in conjunction with those of other grid infrastructures and aim to be as simple and generally applicable as possible. For a community like WLCG, it is critical that common or similar policies be in place across the various infrastructures to enable the required interoperation.

Security is also built into EGEE's middleware. Today's production grids use an extended version of the VO model that includes the ability to define subgroups and roles of VO members more dynamically. The VO Membership Service is a gLite software component that provides this capability by adding extensions to members' X509 proxy certificates to describe them.

The gLite security infrastructure involves sophisticated tools for VO management and local authorization and is currently being integrated with upcoming organization membership services via Shibboleth (<http://shibboleth.internet2.edu>). The information system is based on hierarchical LDAP servers and the accounting system uses the OGF defined usage records, facilitating interoperability with other infrastructures.

Condor and GT2 Grid Resource Allocation Management (currently being updated to GT4 GRAM) provide access to compute resources, work on an interface compliant with the OGF High-Performance Computing Basic Profile (HPC-Profile) and OGF Basic Execution Service (BES) is ongoing (<https://forge.gridforum.org/sf/projects/ogsabes-wg>), and EGEE has standardized the storage resource manager (SRM) interface,⁷ for which a number of production-level implementations are available. GridFTP handles data transfer.

Security coordination emerged out of distributed efforts in operating large-scale infrastructure services.⁸ In the case of EGEE, the operational security activities depend on central coordination and individual local security efforts.

Self-organization

Self-organization describes the inner workings of a complex system and can be understood as "the mechanism that drives the creation of new structures."⁶ Although there is a temptation to impose a consistent structure to facilitate the functioning of complex infrastructures, self-organization often emerges as an inherent force to create new structures because of the functional, disciplinary, and cultural diversity distributed across space and time.

Coordination. Grid management oversight and grid-level monitoring have ensured coordination within EGEE in the past, and it will be achieved through automation and SLAs in the future. EGEE's general strategy is to optimize support activities to reduce the overall level of effort required to manage a sustainable infrastructure. In an era of national grid infrastructures and European-level coordination, it is clear that the present model of grid management oversight is not suitable for the long term. Early experience in the EGEE project has shown the value of distributed operations teams at several levels.

The concept of ROCs as a distributed management team has worked well, providing effort to cover the operational oversight and ensuring the dissemination of knowledge

and expertise. At a finer-grained level, several ROCs themselves are also distributed teams with similar benefits. These ROCs share overall responsibility for the infrastructure on a rotating basis. Therefore, the relationships both within VOs and among ROCs are dynamic.

EGEE's experience managing sites has also made it clear that grid-level monitoring, while vital in the project's earlier stages, must evolve to ensure that resource site managers receive monitoring results directly rather than waiting for grid-level operators to open trouble tickets. Lateral communication rather than hierarchical management is key.

In addition, improvements in grid service management and monitoring must help the site and service managers provide a robust and reliable service with a minimum of external intervention and a maximum of internal self-organization. This strategy is important for ensuring site reliability as well as increasing the scale of the infrastructure without additional staff, eventually reducing the level of effort at the grid oversight level.



For a production infrastructure, reliability and scalability are more valuable than exploitation of the latest advances, which need time to mature.

EGEE has taken actions to address these issues. The most important was setting out a clear automation strategy. A collaboration between EGEE and other infrastructures is working to improve monitoring tools and investigate requirements for increasing the automation of alarms and tools needed to support operations, which will increase reliability, and for verifying SLAs. A guiding principle is to push information and responsibility for proactivity as close to the service itself as possible to ensure fast response. This will reduce the need for higher-level oversight and hopefully turn that role into one of monitoring service metrics such as accounting, site and service reliability, and performance.

EGEE's Operations Coordination Center is establishing SLAs with the ROCs to fully define their required level of commitment, which might differ among centers. It is also responsible for gLite distribution; the ROCs help individual sites install and configure the middleware.

Flexibility. The gLite middleware is released with a business-friendly open source license, allowing both academic and commercial users to download, install, and even modify the code for their own purposes. The grid services use a service-oriented architecture, which facilitates interoperability and makes it easy

to complement gLite services with common application-specific services such as metadata catalogs and metaschedulers.

For a production infrastructure, reliability and scalability are more valuable than exploitation of the latest advances, which need time to mature. EGEE is moving toward Web services that adhere to WS-Interoperability recommendations wherever possible. To achieve the reliability and scalability required to support its workloads, EGEE developers have applied a strict software process involving several stages of testing. This process, which has been modeled after industry-strength processes, includes software configuration management, version control, defect tracking, and an automatic build system.

Europe has invested heavily in e-Science both at the national and regional levels, with impressive results. With strong support from the European Commission, it has become a world leader in the field of grid technology. This technology has become a fundamental component of e-Science. A fast-growing number of communities are now adopting grids, and many are already relying on this technology to achieve their missions.

As the VOs established by scientific communities progress from testing their applications to more routine usage, it becomes increasingly urgent to maintain reliable and adaptive grid infrastructures, independent of project funding cycles. Without such continuity, such communities will hesitate to rely on this new computing paradigm, potentially jeopardizing existing investments and the leading position achieved.

Resource provisioning is a difficult problem to address. Most of the resources made available in the large production grid infrastructures are funded by specific application communities such as WLCG or provided by general e-Science funds in a country, primarily for the use of that nation's research community. To be self-sustaining, grid infrastructure must be able to attract new communities willing to add their own resources to the general pool by improving ease of use and lowering the learning threshold.

Driven by the European research community's needs, a proposed European Grid Initiative (<http://web.eu-egi.eu>) is expected to enable the next leap in grid infrastruc-

ture development, supporting collaborative scientific discoveries in the next decade. Although EGEE has been successful, it is by no means the only model. Future developments will continue to address ongoing complexity and new challenges. **□**

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