

SCE: Grid Environment for Scientific Computing*

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Abstract. Over the last few years Grid computing has evolved into an innovating technology and gotten increased commercial adoption. However, existing Grids do not have enough users as for sustainable development in the long term. This paper proposes several suggestions to this problem on the basis of long-term experience and careful analysis. The Scientific Computing Environment (SCE) in the Chinese Academy of Sciences is introduced as a completely new model and a feasible solution to this problem.

Keywords: Grid, scientific computing, PSE.

1 Introduction

This paper begins with this short introduction. In the second part, a overview of several large Grid projects and its applications (and application Grids) is given, followed by a discussion of existing problems of those Grids, including EGEE, TeraGrid, CNGrid and ScGrid etc. The third part mainly talk about the Scientific Computing Environment (SCE), what it is, why it is important and how it works. The following part introduces applications build upon SCE and how scientists benefit from this integrated environment. The paper ends with final conclusions and future work.

2 Grid Computing Overview

2.1 Grid Computing

Grid computing has been defined in a number of different ways, especially when it's getting increased commercial adoption. People from scientific and research area do not have the same understanding with others from company like IBM,

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Oracle, Sun, etc. However, there is a consensus that Grid computing involves the integration of large computing resources, huge storage and expensive instruments, which are generally linked together from geographically diverse sites.

2.2 Well-Known Grid Projects

Over the last few years, since it was started at Argonne National Labs in 1990, Grid computing has evolved rapidly. Many national Grids, even multi-national Grids are funded to build collaboration environment for scientists and researchers.

EGEE. The Enabling Grids for E-scienceE (EGEE) project brings together scientists and engineers from more than 240 institutions in 45 countries world-wide to provide a seamless Grid infrastructure for e-Science that is available to scientists 24 hours-a-day. The EGEE project aims to provide researchers in academia and industry with access to major computing resources, independent of their geographic location. The first period of the EGEE project was officially ended on the 31 March 2006, and EGEE II was started on 1 April 2006.

The EGEE Grid consists of 41,000 CPU available to users 24 hours a day, 7 days a week, in addition to about 5 PB disk (5 million Gigabytes) + tape MSS of storage, and maintains 100,000 concurrent jobs. Having such resources available changes the way scientific research takes place. The end use depends on the users' needs: large storage capacity, the bandwidth that the infrastructure provides, or the sheer computing power available.

The project primarily concentrates on three core areas:

- To build a consistent, robust and secure Grid network that will attract additional computing resources.
- To continuously improve and maintain the middleware in order to deliver a reliable service to users.
- To attract new users from industry as well as science and ensure they receive the high standard of training and support they need.

Expanding from originally two pilot scientific application fields, high energy physics and life sciences, EGEE now integrates applications from many other scientific fields, ranging from geology to computational chemistry. Generally, the EGEE Grid infrastructure is for scientific research especially where the time and resources needed for running the applications are considered impractical when using traditional IT infrastructures.

TeraGrid. TeraGrid is one of the world's largest, most comprehensive distributed cyberinfrastructure for open scientific research. TeraGrid integrates high-performance computers, data resources and tools, and high-end experimental facilities around USA through high-performance network connections. Currently, TeraGrid resources include more than 750 teraflops of computing capability and more than 30 petabytes of online and archival data storage, with rapid access and retrieval over high-performance networks.

A TeraGrid Science Gateway is a community-developed set of tools, applications, and data collections that are integrated via a portal or a suite of applications. Gateways provide access to a variety of capabilities including workflows, visualization, resource discovery, and job execution services.

Science Gateways enable entire communities of users associated with a common scientific goal to use national resources through a common interface. Science Gateways are enabled by a community allocation whose goal is to delegate account management, accounting, certificates management, and user support to the gateway developers.

TeraGrid is coordinated through the Grid Infrastructure Group (GIG) at the University of Chicago, working in partnership with the Resource Provider sites.

CNGrid. China National Grid (CNGrid) is a key project launched in May 2002 and supported by the China National High-Tech Research and Development Program (the 863 program), and a testbed for the new information infrastructure which aggregates high-performance computing and transaction processing capability. CNGrid promotes the national information construction and the development of relevant industries by technical innovation.

Ten resource providers (also known as grid nodes) from all around China join CNGrid, contribute more than 18 teraflops of computing capability. CNGrid has equipped with self-made grid-oriented high performance computers (Lenovo DeepComp 6800 in Beijing and Dawning 4000A in Shanghai). Two 100-teraflops hpc is being built and will be installed before the end of 2008. Hpc of 1000-teraflops will be built and installed in the near future.

Through the first five years of building, CNGrid has effectively supported many scientific research and application domain, such as resource and environment, advanced manufacturing and information service.

CNGrid is coordinated through the CNGrid Operation Center at Supercomputing Center of Chinese Academy of Sciences. CNGrid Operation Center is established in September 2004 and works with all CNGrid nodes. CNGrid Operation Center is responsible for system monitoring, user management, policy management, training, technical support and international cooperation.

ScGrid. In Chinese Academy of Sciences, construction of supercomputing environment is one of the key supporting area. To build the e-Science infrastructure and make the best of advantage of the supercomputing environment, the CAS has clear and long plans on Grid research and the construction of Scientific Computing Grid (ScGrid).

ScGrid has provided users a problem solving environment based on Grid technology, which is a generic Grid computing platform. ScGrid has supported typical applications from Bioinformatics, Environmental Sciences, Material Sciences, Computational Chemistry, Geophysics etc.

There are other well-known Grid projects like e-Science from UK, NAREGI from Japan and K*Grid from Korea.

2.3 Analysis of Existing Grids

The emerging Grid technology provide a Cyberinfrastructure for application science communities. In UK and China, another word e-Science is used more often when talk about Grid technology. Both characterizations regard Grid as the third basic way to scientific research, and the difference is that ‘Cyberinfrastructure’ focuses on method of scientific research while ‘e-Science’ emphasizes prospect and mode of future research.

All grids are driven by applications in nature, or built for specific applications. Demands from users and applications do exist that can be concluded from above description. Scientific research can be done in a faster and more efficient way by using Grid technology, which has been proven by above Grids.

However, Grids, especially production Grids still need to find more users and arouse more users’ interest. Grids and Grid applications need more active engaged domain scientists. As a example, in the TeraGrid annual report for 2007 [1], the milestone of 300 Science Gateway users was delayed by six months (from month 18 to month 24).

In our experience as the China National Grid Operation Center in the past four years, most of the users’ complaint are:

1. the usability and stability are not enough for daily use;
2. the integrated applications do not cover their needs;
3. the Grid portal is not as convenient as their SSH terminal.

There are a number of issues at stake when we talk about Grid and its value for users, which are also the reasons that users want to choose Grid:

1. Can Grid reduce time of computation and/or time of queuing? This is essential when a user like to choose a alternative and new method (like Grid) to finish her work. Unfortunately, Grid itself is not a technology to make a computation finished faster. But Grid often consists of more than one computation nodes, when a job is submitted, a ‘best’ destination node (faster or less busy one, due to the scheduling policy) could be selected to finish the job, without awareness of the user. So under many conditions, a computation job could finished earlier in Grid.
2. Is it free of charge to use Grid? Users will be very happy if it is true. Furthermore, if the computation (CPU cycle) is also free while using Grid, otherwise not, they will certainly love Grid. It is not good in the long term, however, because any new technology including Grid could not last long if it totally depends on free use.
3. Can Grid give users wonderful experience? There are some user like new things, beautiful and well-designed UI, convenient drag’n’drop mouse manipulation. Users need more choices to select their most familiar and comfortable way to access Grid resources, i.e. via a Grid portal or traditional terminal, from a Linux workstation or a Windows laptop.
4. Apply once, run anywhere in Grid. Many users have accounts on several HPCs, they always need to apply new account on each HPC. In Grid, they

can apply only once, a Grid account, to have local account on each Grid node. This could save much time.

From above analysis, resource sharing and scheduling is still the key value of Grid for users. Each Grid user must have a local account on every single Grid node, and each submitted job must be delivered to a specific Grid node. This is the basic concept of Grid, while it is sometimes ideal in reality.

In this kind of situation, on the one hand, functions of software need to be improved, on the other hand, operation and management is also a big issue that need more concern.

3 Scientific Computing Environment

In the eleventh five-year plan of the Chinese Academy of Sciences, the construction of supercomputing environment is designed as a pyramidal structure. The top layer is a centralized high-end computing environment, building a one hundred teraflops computer and software support platform. The middle layer is distributed among China, choosing five sub-center and integrating fifty teraflops of computing resource. The bottom layer consists of institutes in the CAS, they can have their own hpcs with different dimensions.

Under this pyramidal layout, based on ScGrid and the work during the tenth five-year plan, Grid computing technology is the best choice for sharing resource and integrating computing power.

3.1 Structure of SCE

Supercomputing Center continues the research and construction of Scientific Computing Grid during the advance of e-Science infrastructure in Chinese Academy of Sciences. To make the best of advantage of the Scientific Computing Environment (SCE), Supercomputing Center provide users a easy-to-use problem solving environment based on Grid technology.

The basic structure of SCE is illustrated in figure 1. In the bottom, there are different high performance computers and visualization workstations that consists of hardware layer. Grid middleware is a abstract and transparent layer that shields the difference of geographical locations and heterogeneous machines in the hardware layer. It also serve as a Grid services provider for upper client tools and portals. Users choose whatever client tools or portals to access Grid resources as they like.

3.2 Features of SCE

Integrated and Transparent. In the integrated scientific computing environment, computing jobs are scheduling among all computing nodes. Jobs can be submitted to a specified node or a node selected automatically. Large scale and long-time jobs can be scheduled to the top or middle layer with more powerful computing capability. Other small or short-time jobs will be scheduled to the

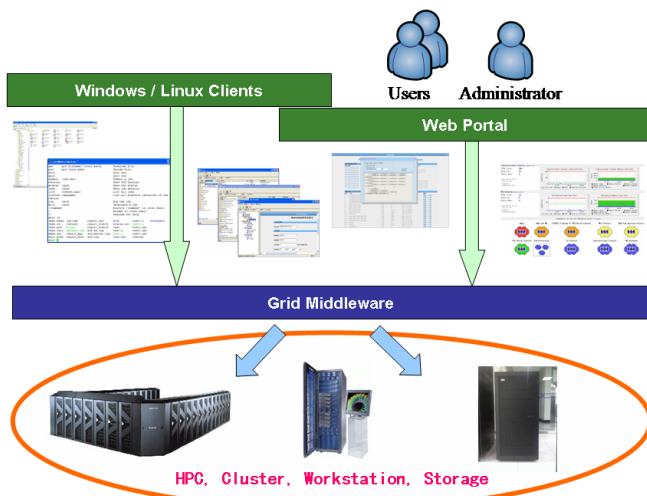


Fig. 1. Basic structure of SCE

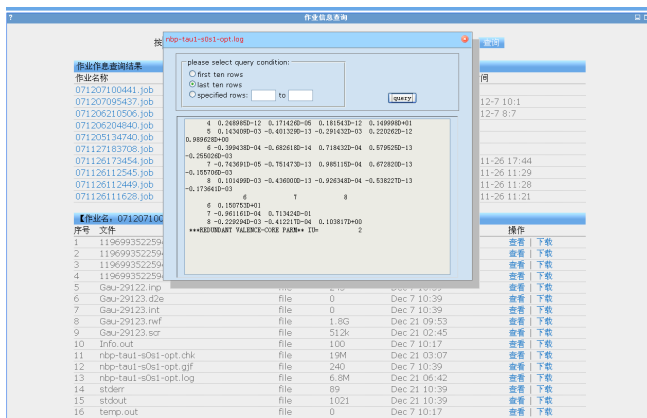


Fig. 2. Submitting a Gaussian Job in Grid portal

middle or bottom layer. When all comes to all, the utilization of high performance computers are maximize. On the other hand, users do not need to logon to different nodes. They can login once, and use all the nodes. All are transparent to users as a larger computers.

Flexible and easy-to-use. Users can choose to use either web portal or client tool. In web portal (see figure 2), normal jobs can be submitted, job status can be checked, intermediate output can be viewed, and final result can be downloaded. In figure 2, the status of a running Gaussian job is listed and the instant output of intermediate file is dumped in the center window. In client tools, in addition, files can be transferred in multi-thread. Remote file systems on all Grid nodes

can be mounted locally in the Windows explorer. Directories and files of three remote hpcs are listed concurrently in the left tree view of Windows explorer. Remote file operations are as easy and normal as doing locally.

Lightweight and scalable. The source code of SCE middleware is mainly written in C and Shell script, the core code is around ten thousand lines. So it is very easy to deploy and setup. Also, the modular design make it easy to scale, new functions can be easily added.

3.3 Applications Based on SCE

Vitua Laboratory of Computational Chemistry. VLCC is a very successful example of the combination of Grid technology and specific application. VLCC is established in 2004, which aims at building for computational chemistry a platform of research, communication between scientists, training for newbies and application software development. Until now, there are more fifty members from universities and institutes that join the virtual laboratory. Many software are shared between those members, from commercial software, i.e. Gaussian 2003, ADF 2004, Molpro and VASP, to free software CPMD, GAMESS, and GROMACS etc. Scientists also share software developed by themselves with others, including XIAN-CI by Professor Zhenyuan Wen from North West University of China, CCSD and SCIDVD by Professor Zhigang Shuai from Institute of Chemistry of CAS, 3D by Professor Keli Han from Dalian Institute of Chemistry Physics. The success of VLCC arouses inspiration of researchers from other application domains. Similar virtual laboratories are planned.

4 Conclusions and Future Work

Grid computing involves the integration of large computing resources, huge storage and expensive instruments. Over the last few years, Grid computing has evolved rapidly. Many national Grids, even multi-national Grids like EGEE, TeraGrid, CNGrid are built.

The Scientific Computing Environment (SCE) in the Chinese Academy of Sciences is a completely new model which put emphasis on consistent operation and management, and versatile accessing method to meet users' demand. Successful applications in the SCE integrated environment show it is a feasible solution to this problem.

Also more applications are being integrated in SCE.

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References

1. Catlett, C., et al.: TeraGrid Report for CY 2006 Program Plan for 2007 (January 2007)
2. Foster, I., Kesselman, C.: *The Grid: Blueprint for a New Computing Infrastructure*. Morgan Kaufmann, San Francisco (1998)
3. Foster, I., Kesselman, C., Nick, J., Tuecke, S.: *The Physiology of the Grid: An Open Grid Services Architecture for Distributed Systems Integration* (January 2002)
4. von Laszewski, G., Pieper, G.W., Wagstrom, P.: *Gestalt of the Grid*, May 12 (2002)
5. Yin, X.-c., Lu, Z., Chi, X., Zhang, H.: The China ACES iSERVO Grid Node. *Computing in Science & Engineering (IEEE)* 7(4), 38–42 (2005)
6. Zhu, J., Guo, A., Lu, Z., Wu, Y., Shen, B., Chi, X.: Analysis of the Bioinformatics Grid Technique Application in China. In: *Fourth International Workshop on Biomedical Computations on the Grid*, May 16-19, 2006. Nanyang Technological University, Singapore (2006)
7. Sun, Y., Shen, B., Lu, Z., Jin, Z., Chi, X.: GridMol: a grid application for molecular modeling and visualization. *Journal of Computer-Aided Molecular Design(SCI)* 22(2), 119–129 (2008)
8. Wu, H., Chi, X.-b., Xiao, H.-l.: An Example of Application-Specific Portal in Web-based Supercomputing Environment. In: *International Conference on Parallel Algorithms and Computing Environments (ICPACE)*, October 8-11, 2003, pp. 135–138 (2003)
9. Haili, X., Hong, W., Xuebin, C.: An Implementation of Interactive Jobs Submission for Grid Computing Portals. *Australian Computer Science Communications* 27(7), 67–70 (2005)
10. Xiao, H., Wu, H., Chi, X.: A Novel Approach to Remote File Management in Grid Environments. In: *DCABES 2007*, vol. II, pp. 641–644 (2007)
11. Dai, Z., Wu, L., Xiao, H.: A Lightweight Grid Middleware Based on OPENSSE - SCE. In: *Grid and Cooperative Computing*, pp. 387–394 (2007)
12. <http://www.863.org.cn>
13. <http://www.cngrid.org>
14. <http://www.eu-egee.org>
15. <http://www.teragrid.org>
16. <http://www.sccas.cn>
17. <http://www.scgrid.cn>
18. <http://www.top500.org>