GRINKO - Grid e-Infrastructure and Networking with Kosovo

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Grid Computing offers an efficient way of utilization of computer resources for research computations. In contrast to common localized strategies like workstations, Grid Computing follows a decentralized approach. The computer resources are spread over a larger region, country, or continent. Members of the Grid start their programs on their own sites and these jobs are scheduled somewhere on the Grid. The actual location of execution is of no interest.

A computational grid is a computing environment which enables the unification of geographically widely distributed computing resources into one big (super)computer [1]. The individual computing resources commonly consist mostly of computer clusters or several individual computers, which are interconnected by a high-speed wide area network. The grid is a computer system which is, at this moment, primarily intended for supporting e-Science, however the technology itself is very adaptable for a very wide area of present and future computer use. The major goal of a grid is to enable the clustering and unification of distributed computing and data processing resources. This is done to accumulate and coordinate as much computing power as possible and make it available for use by applications, which have a particularly high demand for computing resources. Examples of scientific applications greatly benefiting or even necessitating a grid are from the fields of particle physics, climate analysis, biomedical research, meteorology etc.

The South Eastern European region had brought up a number of Grid activities. Main topic of the Grinko Project was to built up a pilot grid environment in Kosovo.
The SEE-GRID

The SEE-GRID infrastructure contains computational and storage resources for scientific application, which are made available by more than fifteen partners from different countries in South East Europe. An illustration of the distributed nature of the SEE-GRID is given in Figure 1. Currently, the SEE-GRID provides more than 35 clusters with a total number of more than 2000 CPUs and a storage capacity exceeding 400 TB [2]. This Grid infrastructure is built using the gLite middleware [3], which provides Web Service APIs for most of its services, and also provides new types of services, such as the gLite WMS, gLite FTS, AMGA, etc. The middleware also improves the reliability and scalability of other services.

Figure 1: The SEE-GRID infrastructure
Each of the SEE-GRID clusters provides the mandatory services [4]:
- Computing element (CE) - provides user access to the grid resources
- Worker nodes (WN) - execute jobs, perform calculations
- Storage element (dCache, DPM or classic SE) - reliable data storage
- MON box (Monitoring and accounting) - monitor the current grid status and report completed jobs and their used resources

- The worker nodes provide the computational resources, while the storage elements provide storage resources
- The set of services, which are not tied to a specific site are called core services. In the SEE-GRID the core services are distributed among partners.

They include:
- VOMS (Virtual organization management system)
- MyProxy
- R-GMA registry/schema server (distributed data-base)
- BDII (provides comprehensive information about the resources)
– WMS (distributes and manages the jobs among different grid sites)
– FTS (file transfer service)
– AMGA (meta data catalog)
The differences and similarities how users can access a grid on the one hand and workstations or PCs on the other hand are shown in Table 1.

<table>
<thead>
<tr>
<th>PCs or workstations</th>
<th>PCs or workstations</th>
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<tbody>
<tr>
<td>Login with a username and password (“Authentication”)</td>
<td>Login with digital credentials; single sign-on (“Authentication”)</td>
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<tr>
<td>Use rights given to user (“Authorisation”)</td>
<td>Use rights given to user (“Authorisation”)</td>
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<tr>
<td>Run jobs</td>
<td>Run jobs</td>
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<tr>
<td>Manage files: create them, read/write, list directories</td>
<td>Manage files: create them, read/write, list directories</td>
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<tr>
<td>Components are linked by a bus</td>
<td>Services are linked by the Internet</td>
</tr>
<tr>
<td>Operating system</td>
<td>Middle ware</td>
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<tr>
<td>One admin domain</td>
<td>Many admin domains</td>
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Table 3: Similarities and differences between a Grid and a PC

Our applications we mention below have been mainly performed on two main grid clusters - BG03-NGCCP and BG04-ACAD which are situated in the Institute for Parallel Processing. The specifications of the grid clusters used in our experiments are:

- The BG03-NGCC grid cluster has 25 worker nodes, which contain 2xIntel Xeon E5430 2.66 GHz Quad Core CPU (total 200 Cores, > 400 KSI2000) with 16 GB RAM on each node.
- The BG04-ACAD has 40 worker nodes with 2xOpteron 2,4 GHz (total 80 cores, >120 KSI2000), 4GB RAM on each node, and a low-latency Myrinet interconnect for MPI jobs.
Partners of the Project

The envolved partners in this project feature high experience in the field of Grid Computing, Computer Administration, Mathematical Modeling, Simulation of Technical Problems. In detail the partners had been:

IuE - Institute for Microelectronics, Technische Universität Wien, Vienna, Austria  http://www.iue.tuwien.ac.at

FTS - Faculty of Technical Sciences, University of Pristina, K. Mitrovica, Kosovo  http://www.ftnkm.info/ftn/pocetna.php

IPP-BAS - Institute for Parallel Processing, Bulgarian Academy of Science, Sofia, Bulgaria  http://www.bas.bg/clpp/en/indexen.htm

FEEIT - Faculty of Electrical Engineering and Information Technologies St. Cyril and Methodius University - Skopje, Macedonia  http://www.feit.ukim.edu.mk

<table>
<thead>
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Objectives

The main objectives of the GRINKO project are:

- To provide specific support actions to assist the establishment of the pilot Grid center in the Faculty of Technical Sciences (K. Mitrovica), University of Pristina (FTS-UP-K.M.). The envisaged training, dissemination and collaboration activities aim to provide the knowledge and ability to use the Grid infrastructure for solving of computationally demanding problems in the field of Technical Sciences. The computer experts comprising the Kosovo team will acquire knowledge to provide Grid support to the electrical engineering, electronic and other local scientific communities with requirements for high performance computing power, as for example are these from ecology and geophysics. The Kosovo partners become the core group working for the enlargement of local Grid infrastructure, attracting more users and applications.

- To establish scientific cooperation and human networking between the research working group from Institute for Microelectronics, Vienna University of Technology (IuE-TU), Faculty of Technical Sciences (K. Mitrovica), University of Pristina (FTS-UP-K.M.), Institute for Parallel Processing of Bulgarian Academy of Sciences (IPP-BAS) and Faculty of Electrical Engineering and Information Technologies in Ss Cyril and Methodius University – Skopje (FEEIT-UKIM).

Grid computing facilitates collaborative development of
applications and sharing of scientific results. The good mix of expertise in Computational Electronics (IuE-TU and FEEIT-UKIM), grid and parallel computing (IuE-TU, IPP-BAS, and FEEIT-UKIM), simulation and design of semiconductor devices (IuE-TU and FTS-UP-K.M.), of the participating teams will produce synergies. The good dissemination and training strategy will allow the spreading of knowledge towards other interested communities.

- To exploit and adapt scientific methods and approaches to computational problems specified by/to the researchers in Kosovo. In accordance with their research interests, these are problems arising in the field of Electronics, Material Science, and Monitoring systems. The project aims to identify a set of interesting computational problems, suitable for Grid computing, implement a Grid strategy for their solution, and achieve novel scientific results by running the codes on the Grid infrastructure, provided by the partners.

**Project Content**

The project contains 4 main activities:

- **WP1** - Administrative and technical management - The goal of this activity is to put in place a management structure and communication mechanisms enabling effective administrative and technical management of the consortium;

- **WP2** – Grid Infrastructure Operation – A pilot grid cluster will be installed in FTS-UP-K.M, using standardized European EGEE Grid middleware – gLite. The other partners will provide the operational support and access to their existing grid clusters;

- **WP3** – Grid applications and user communities support – identifying, developing, testing and deploying grid applications from the area of Computational Electronics;

- **WP4** – Dissemination and Training - addresses dissemination of the research results to conferences,
seminars and organised training events for the Kosovar researchers to use the Grid technologies and Grid application development;

These activities can be summarized as dissemination of the European concept for establishing of Grid infrastructures in all EU countries in order to provide access of grid users to computational resources and storage. Thus, users can develop, test, and deploy on Grid clusters their computational intensives problems arising from different scientific areas.

Achieved Results

During the project period the following main results are achieved:

- Transfer of knowledge – how to install a small grid cluster:
  The installation includes Computer Elements (CE), Storage Elements (SE) and Worker Nodes (WN) as main parts of the cluster. Additionally, on workstations User Interfaces (UI) have to be installed to access the Grid.

- Developing Grid applications:
  Two interesting topics had been chosen of the range of computational electronics, in detail these are (i) Modeling Thermal Effects in Nano-Devices and (ii) Mixed Mode Carrier Transport Modeling.

- Testing these grid applications on the Grid and obtaining first results computed in a parallel way.

- Disseminating of the achieved scientific results on international conferences. The papers had been already submitted and will be published in the near future.

The project results per activity are described in the following:

WP1 - Administrative and technical management
The project homepage and information system is available at http://www.iue.tuwien.ac.at/grinko/Home/index.html
Main objectives of the GRINKO project can be examined at the Bulgarian partner site http://www.grid.bas.bg/site/index.php?page=grinko
Organisation of the meetings and trainings.

All administrative and technical management were done by the project coordinator IuE-TU. It helped to organise all GRINKO meetings and trainings. During the Grinko meetings all activities leaders prepared presentations concerning the progress of the Wps.

Goal was to establish a project management mechanism - using e-mails, creating Web pages, ... in order to exchange information about progress of all tasks. The interim report, final project presentation and final report were also prepared by the coordinator with support from all partners.

WP2 – Grid Infrastructure Operation

A pilot grid cluster was installed in FTS-UP-K.M, using standardized European EGEE Grid middleware – gLite. At Faculty of Technical Sciences of Kosovska Mitrovica, FTS-UP-K.M, the ninth grid site is installed - AEGIS09-FTN-KM currently consisting of 2 nodes running Scientific Linux 4.7, with gLite 3.1.0 with MPI support and storage element of 1TB.

- The hardware consists of the following:
  1 quad core 2.4GHz, 2Gb RAM, 640Gb HDD (Computing Element)
  1 dual core 2.5GHz, 2Gb RAM, 1280Gb HDD (Storage Element)
  2 dual core 2.5GHz, 2Gb RAM, 640Gb HDD (total 4 Worker Nodes)

- Software: Scientific Linux 4.7, gLite middleware

- Public IP addresses had been assigned to these machines and grid host certificates from AEGIS Certification Authority http://aegis-ca.rcub.bg.ac.yu/ had been received.

- IPP-BAS provided access (giving the user grid certificates to partner members http://ca.acad.bg/certs/) to their grid clusters with more than 300 Wns.

The grid cluster AEGIS09-FTN-KM is currently monitored by GStat monitoring system which monitors the global Grid infrastructure: http://egee017.cnaf.infn.it/gstat/AEGIS09-FTN-
Figure 1: AEGIS monitoring of the Grid cluster at the Faculty of Technical Sciences, Kosovska Mitrovica

WP3 – Grid applications and user communities support
The first application (Modeling Thermal Effects in Nano-Devices) has been presented at the meeting in Skopje. During development this application was adapted for Grid submission. For parallelization this application raises hard barriers. If parallelized, the solving technique for this application requires quite hard communication between the different processes. Submitting such processes on a grid, the overall performance will severely decrease. Therefore, this application is only well suited for single job submission. However, for calculating a complete characteristic several single jobs have to be started, which can be done in parallel.

Very well suited for parallelization is a second application: the Mixed Mode Transport Modeling, which considers both coherent and dissipative processes which govern the electron behavior in nanostructures and thus their operation. Due to the very small
device dimensions an interacting electron will highly probably not interact a second time. All interactions can be handled independently and no communication is used during simulation, and, therefore, can be splitted in parallel on the Grid. Finally, after termination of all jobs the data can be collected. A result of such a calculation can be seen in Figure 4.

The application has been fully adapted for the Grid, tested, deployed, and parallelized using MPI. Within this cluster 300 WNs are available.

Typically one Job runs 7-8 hours using 4 WNs. To achieve a whole characteristic hundreds of such jobs are necessary, which may be sent in parallel to the grid. Currently an improvement of the parallel implementation on the Grid is aimed to increase the efficiency.

![Figure 2: Result of one electric simulation. Typically this calculation uses 7 hours on 4 WNs.](image)

Scientific results had been presented on

- 7th International Conference on "Large-Scale Scientific Computations", Sozopol, June 4-8, 2009
- "Grid Computing & Applications in Physics and Mechanics" at "Euro-American Consortium for Promoting
WP4 – Dissemination and Training
During the GRINKO project three meetings for all members had been planned. Additionally, there was a Grid training organized in Belgrade where team members attended. Important dates of the trainings are:

- GRINKO kick-off meeting, Sozopol, Bulgaria, June 11-12, 2008, in conjunction with the 34th International conference AMEE’08, 8-14 June 2008.
- Team members from FTS-UP-K.M. and IPP-BAS participated in the regional training for Grid site administrators in Belgrade, 5-6, March, 2009. This meeting was in collaboration with partners from SEEGRID-SCI projects.
- GRINKO meeting and training, Sofia, Bulgaria, 4-5 April, 2009.

Challenges during the project

At the beginning of the project some diplomatic issues had been clarified for the Kosovar partners. The autonomy of Kosovo had not been accepted by all governments. This was recognized when invitation letters had been rejected by post. However, the Visa formalities for the Kosovo partners had not been a problem. Within one month it was always possible to achieve them.

Buying the hardware for the Faculty of Technical Sciences, Kosovska Mitrovica caused a delay of 2 months. Also obtaining public IP addresses, network connections and grid certificates necessary for building up a Grid posed some hurdles. The training in Sofia was moved to the beginning of April. In between members of the GRINKO project participated in the regional training for Grid site administrators in Belgrade, 5-6, March 2009.
Afterwards the hardware in Kosovo had been set up and during
the meeting the emphasis was set to the development, testing,
and deployment of the Grid applications. During the training also
some limitations for parallelization had been recognized. Commu-
nicational intensive jobs are not well suited to spawn them over a
grid. In this case it is advantageous to submit many single jobs on
the Grid in order to achieve a complete characteristic.

Future Plans

Achieved Grid certificates are valid for one year ahead. The testing
of the installation of the Grid cluster in the Faculty of Technical
Sciences – K. Mitrovica (FTS-UK-K.M.) continues in order to solve
some problems and to prepare it to join in SEEGRID Infrastructure.

http://goc.grid.sinica.edu.tw/gstat/seegrid/

Future plans of the Bulgarian partner include the preparation of
new a national project and will involve partners from GRINKO. Future bilateral cooperation
between GRINKO partners are aspired for the future. New calls
under FP7 and other regional initiatives are examined.

W. Cahn, M. C. Flemings, E. J. Kramer, and S. Mahajan (eds.) Encyclopedia of Materials:
simulation on the grid, LNCS 4818, 461–469 (2008), Springer-Verlag.