Serbian participation in Grid computing projects

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Pan-European EGEE, regional SEE-GRID, and Serbian AEGIS eInfrastructures have a common aim - provision of processing and storage services for eScience research. Serbia participates in these projects, by developing new applications, providing computing and storage resources and advanced services to scientific, research and development communities, fostering collaboration, and attracting a wide range of new users to the Grid. We give an overview of our activities and main achievements in Grid computing projects.

1. Introduction to Grid computing

Science is becoming largely digital - it needs to deal with ever increasing amounts of data and computational needs. Numerical simulations become more detailed, experimental science uses more sophisticated sensors to make precise measurements, and shift from the tradition of individuals-based science work towards more collaborative models now starts to dominate.

Computing resources and services able to support needs of such a new model of scientific work are available at different layers: local computing centers, national and regional computing centers, and European supercomputing centers. The gap between needs of various user communities and computing resources able to satisfy their requirements is addressed by introduction of Grid technology on the top of pan-European academic network.

Computing Grids are conceptually not unlike electrical grids. In an electrical grid, the wall outlets allow us to link to and use an infrastructure of resources, which generate, distribute, and bill for electrical power. When we connect to the electrical grid, we do not need to know details on the power plant currently generating the electricity we use. In the same way Grid technology uses middleware layer to coordinate and organize into one logical resource a set of available distributed computing and storage resources across a network, allowing users to access them in a unified fashion. The computing Grids, like electrical grids, aim to provide users with easy access to all the resources they need, whenever they need them, regardless of the underlying physical topology and management model of individual clusters.

Grids address two distinct but related goals: providing remote access to information technology (IT) assets, and aggregating processing and storage power. The most obvious resources included in Grids are processors (CPUs), but Grids also can encompass various sensors, data-storage systems, applications, and other types of resources. One of the first commonly known Grid initiatives was the SETI@HOME project [1], which solicited several millions of volunteers to download a screensaver, which was able to use idle processor time to analyze the astronomical data in the search for extraterrestrial life.

Europe has played a leading role in Grid technology development, starting with the EU DataGrid project [2] and related efforts under the Framework Programme 5. After this proof of concept, demonstrating the potential impact of Grid technologies on European science and industry, a first large scale production Grid infrastructure was deployed by the Enabling Grids for E-SciencE project [3] (EGEE), and its operation was further consolidated in its second phase (EGEE-III). Current phase of EGEE programme, EGEE-III project in close collaboration with pan-European network provided by GÉANT2 [4], National Grid Infrastructures (NGIs), and the European Grid Initiative Design Study project [5] aims to

prepare the transition towards a sustainable Grid infrastructure after the current set of short-term projects is completed.

In the past five years the European Commission has funded through a number of targeted initiatives activating of new user communities and enabling collaborative research across a number of fields in order to close existing technological and scientific gaps, and thus bridging the digital divide, stimulating research and consequently alleviating the brain drain in the less-developed regions of Europe. This was especially successful in the South-East Europe (SEE), where a number of such initiatives show excellent results. The SEEREN [6] (SEE Research and Education Networking initiative) project, through its two phases, established the SEE segment of the pan-European GÉANT network and successfully connected the scientific communities in the region. Currently, the SEE-LIGHT project is working towards establishing a dark-fibre backbone that will interconnect most national research and education networks in the region. In the Grid arena, the SEE-GRID [7] (South-East European GRid eInfrastructure Development) project, similarly through its two phases, has established a strong human network in the area of scientific computing and has set up a powerful regional Grid infrastructure, attracting large number of applications from diverse fields from countries throughout the South-East Europe. The third phase of SEE-GRID programme (SEE-GRID-SCI) aims to have a catalytic and structuring effect on a number of SEE user groups, with a strong focus on the key seismological, meteorological, and environmental communities.

Inline with the European and regional vision of paving the way towards a long-term sustainable European Grid Initiative, Academic and Educational Grid Initiative of Serbia [8] (AEGIS) is bringing together under one umbrella at the national level all interested parties involved in provisioning and using of Serbian research computing infrastructure. Institute of Physics Belgrade [9] (IPB) coordinates AEGIS initiative through its Scientific Computing Laboratory [10] (SCL). AEGIS and IPB participate in pan-European EGEE and regional SEE-GRID programmes, integrating Serbian research and education communities to European Research Area (ERA), and promoting and implementing European and regional Grid activities at the national level.

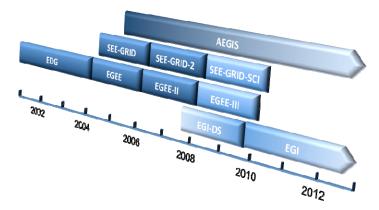


Fig. 1. Roadmap to a sustainable Serbian Grid infrastructure

2. Grid projects relevant for Serbia

Pan-European EGEE, regional SEE-GRID, and Serbian AEGIS eInfrastructures have a common aim - provision of processing and storage services for eScience research. Serbia actively participates in these projects (Fig. 1.), sharing national computing and storage resources with other countries from the SEE region and from the Europe, fostering collaboration and providing advanced computing services and capabilities to Serbian researchers, as well as to other researchers using the shared Grid eInfrastructure.

2.1. EGEE programme

The EGEE programme, which is built on top of national and thematic Grid efforts, as well as the pan-European network provided by GÉANT2 and the NRENs (National Research and Education Network), aims to deliver Grid technology to many scientific disciplines and to users with widely varying levels of computing expertise located all over the globe. Since the beginning of EGEE, there has been a substantial expansion in the use of the infrastructure by a broad range of scientific applications. Scientists are clustered into Virtual Organizations (VOs), a framework to conduct collaborative research and gain access to shared computing and data resources. EGEE provides a variety of services to scientists, ranging from training and user support, to the software interfaces and APIs necessary to access the resources. The number of EGEE VOs supported now exceeds 250, and about 150,000 jobs/day are routinely executed worldwide on the eInfrastructure comprising more than 280 sites in over 55 countries. These applications deal with more than 100 PB of data made available on the EGEE data storage resources, which sees routine aggregated data transfers of more than 1GB/sec. The number of scientists benefiting from EGEE has grown to over 15,000.

Life Sciences and High Energy Physics now depend on the EGEE Grid infrastructure, which is an essential and crucial part of their large-scale data processing. Other disciplines, notably astrophysics, earth sciences, computational chemistry, and fusion (to name but a few) are also increasingly using EGEE resources for production and processing of data. Close relations are established with a number of collaborating projects extending the infrastructure and applications support to more disciplines. Through these collaborating projects and interoperability efforts with related non-European infrastructures, EGEE contributes to the establishment of a seamless worldwide computing infrastructure. Continuous advancements of EGEE's relations with business have contributed significantly to the growing uptake of Grid technologies in the commercial sector, with first prototype service providers appearing on the market and several sectors deploying enterprise Grid infrastructures.

Given the success of the EGEE programme, it is essential to build on its achievements and prepare the transition towards a sustainable infrastructure in the future. EGEE-III project, undertaken in close collaboration with National Grid Infrastructures (NGIs) and the European Grid Initiative Design Study (EGI_DS) project are designing a conceptual set-up of a new organizational model, based on NGIs such as the UK National Grid Service [11] (NGS), D-GRID [12] in Germany or AEGIS in Serbia for a sustainable pan-European Grid infrastructure. EGEE-III and all NGIs work closely with EGI_DS to transfer their experience in operating large-scale international Grid infrastructures, ensuring the development of a viable model in EGI_DS. Based on the plans to be produced by EGI_DS, EGEE-III will, in its second year, start implementing the required structural changes to allow a seamless transition to the European Grid Initiative (EGI) model, while ensuring the continued provision of the Grid service.

2.2. SEE-GRID programme

The SEE-GRID programme through its two phases has established a strong regional human network in the area of scientific computing, has set up a powerful regional Grid infrastructure, and attracted a number of applications from diverse fields from countries throughout the South-East Europe. Current phase of SEE-GRID programme, SEE-GRID-SCI (SEE-GRID eInfrastructure for regional eScience) involves three strategic international scientific communities (seismology, meteorology, environmental protection) and thus further stimulates the use and expansion of the existing regional eInfrastructure and its services, and capitalize on the existing human network to further strengthen scientific collaboration and cooperation among participating SEE communities in the area of eInfrastructures.

The inclusion of the new scientific communities and the expansion of the infrastructure in terms of both size and geographical spread, together with a set of coordinated actions aimed at strengthening the National Grid Infrastructures in the region, will ensure that at the end of the project each country in the region will be ready to join the long-term, sustainable European Grid Initiative as a full-fledged peer.

2.3. AEGIS programme

Academic and Educational Grid Initiative of Serbia (AEGIS) was established in 2005 to coordinate efforts on developing academic and educational high performance computing facilities (e.g. computers, storage, networks, instruments, and visualization resources) in Serbia, and help to integrate them in the AEGIS infrastructure. One of the major AEGIS tasks is dissemination and training activities organization, and help to Serbian research communities in developing and production use of applications on the AEGIS eInfrastructure.

AEGIS is also focal point in Serbia for facilitation of wider participation of AEGIS members in Framework Programme 7 and other international Grid projects, coordination of fund raising efforts to improve AEGIS infrastructure and human resources, creation of national Grid development policy, and lobbying for its position within an overall research agenda.

3. Serbian Grid resources – AEGIS eInfrastructure

The Serbian Grid infrastructure [13] consists of nine Grid sites (Fig. 2.), comprising from tens to hundreds of computing nodes and disk-based storage elements ranging from several hard disks to tens of terabytes. Apart from computing and storage resources, core Grid services which enable seamless access to all resources are provided to national users. AEGIS sites are running Scientific Linux operating system [14] and the latest version of the EGEE gLite middleware. Beside standard serial tasks, sites are optimized and heavily tested for parallel processing mode using MPICH framework [15]. The resources are fully dedicated to national and international Grid communities within AEGIS, SEE-GRID and EGEE projects.

The first Grid site in Serbia **AEGIS01-IPB-SCL** is installed at the Scientific Computing Laboratory of the Institute of Physics Belgrade. This Grid site is a set of 89 worker nodes (2 x quad core Xeon E5345 on 2.33 GHz with 8GB of RAM) and 15 service nodes (Xeon based nodes). AEGIS01-IPB-SCL, as the largest, is the Tier-0 site in the Serbian Grid infrastructure, providing all core services and managing national AEGIS Virtual Organization. All computing and core services nodes at AEGIS01-IPB-SCL Grid site are interconnected by the star topology Gigabit Ethernet network through three stacked high-throughput Layer 3 switches, each node being connected to the switch by two Gigabit Ethernet cables in channel bonding. In terms of storage resources, AEGIS01-IPB-SCL provides 27 TB of disk space to the Grid community.

Belgrade University Computer Centre [16] (RCUB) hosts **AEGIS02-RCUB** grid site. The site consists of 14 nodes with 2.0 GHz AMD Sempron CPUs with 1GB of RAM. The Storage Area Network (SAN) cluster is connected to the storage element via NFS. The Laboratory for Electronic Design Automation [17] (LEDA) of the Faculty of Electronic Engineering, University of Nis has deployed **AEGIS03-ELEF-LEDA** site. The site capacity is currently being extended to 64 CPUs (Intel Xeon Quad-core 2.4GHz, with 12MB L2 cache and 4GB RAM per node), and the site storage capacity is 2TB.

The site **AEGIS04-KG** is installed at the Bioengineering Research and Development Center [18] of the University of Kragujevac since June 2006. It consists of 42 CPU cores with the total RAM of 40GB. The School of Electrical Engineering [19] of the University of Belgrade hosts **AEGIS05-ETFBG** Grid site. It consists of 30 nodes (AMD 2600+ Sempron CPUs), with 1GB RAM and 80 GB of disk space at the storage element.

AEGIS07-IPB-ATLAS is the second site hosted by the Institute of Physics Belgrade, and is based on 128 Intel Xeon processors with 32-bit architecture and the total of 96GB of RAM. The site supports several virtual organizations, but is mainly dedicated to the ATLAS VO community of the CERN LHC experiment. Another site at Institute of Physics Belgrade, **AEGIS08-IPB-DEMO**, is used purely for educational/training purposes. It is based on Xen virtual machines deployed on a single node with two Intel Xeon Quad-core CPUs with 16 GB of RAM. It is used in various training events for demonstration of installation and configuration of different Grid services.

With the support of the GRINKO project [20], **AEGIS09-FTN-KM** Grid site has been established in Kosovska Mitrovica at the Faculty of Technical Sciences [21] of the University of Pristina. This site consists of four Quad-core CPU computing nodes.



Fig. 2. Overview of the Serbian Grid infrastructure

4. AEGIS applications

Apart from establishing a reliable national Grid eInfrastructure, one of the most important results of Serbian Grid activities is the production use of the pan-European EGEE, regional SEE-GRID and national AEGIS infrastructures by a large number of diverse applications developed by Serbian researchers. The user activities drive the evolution of Grid technology through specific, challenging applications, and demonstrate that these infrastructures provide viable computing services for many scientific communities. AEGIS applications require, in particular, that the Grid middleware performance and core Grid services scale with the growth of the infrastructure, and have additional requirements for high-level services. Here we will describe the most used applications, developed and gridified by the Serbian Grid community.

The grid-enabled **Volumetric Image Visualization Environment (VIVE)** is an interactive analysis tool for 3D medical images, facilitating diagnosis, surgical planning, therapy evaluation, and remote 3D examination. It improves understanding of complex anatomies by providing an interactive three-dimensional environment with simple Web-based user interface. The lightweight Java/VRML client enables user interaction and 3D rendering within a Web browser. The user interacts with the visualization server running on the grid through the specialized portal responsible for job submission and communication with server jobs. The grid provides computing and storage resources, as well as access methods required for volumetric data processing.

Grid-based computational model of realistic blood flow in a section of artery -**Parallel Blood Flow Simulation (PBFS)** - improves diagnosis and treatment of health problems such as aneurysms and wounds to artery vessel walls. Systems of equations describing fluid and wall behavior are numerically simulated in Center for Scientific Research of Serbian Academy of Science and Art and University of Kragujevac with parallel computational software environment for solving equations using finite element analysis. These systems include Navier-Stokes and incompressible fluid equations coupled through boundary conditions to the deformable wall motion using fluid-structure interactions.

Gridified version of the Path Integral Monte Carlo **SPEEDUP** code presents efficient and reliable tool for calculating basic properties of matter, such as free energy, energy spectra, probability amplitudes, low and high temperature properties etc. Until recently the best available result for partition functions of a generic N-fold discretized theory led to a $1/N^4$ convergence. In a series of papers developers fro SCL have investigated the dynamical implications of stochastic self-similarity by studying the relation between discretization of path integrals with different coarseness. This has resulted in a systematic analytical procedure that is used to reduce path integral error to $O(1/N^p)$ for integer p as high as 35 for onedimensional theories and 10 for general many-body models. This reduction of error brings about a substantial increase in the speed of calculation of path integrals.

The grid-enabled simulation of planetary system formation - **SOLAR** - presents an effective model of planetary accretion. It provides possibility to simulate the formation of planetary systems starting from as many as $N=10^{12}$ initial particles, and to investigate properties of condensates, including the distribution of their masses, spins, and radial distributions. It is also possible to investigate evolution of these properties during the condensation process, and to uncover sensitivity of key features of such systems on initial conditions.

Grid-based simulation of the compaction of granular materials – **COMPACTION** - is event driven method to simulate compaction processes in two-dimensional vibrating boxes. Event driven method is modification of molecular dynamics approach since the simulation increments from collision event to collision event rather than incrementing at a specified time. Inelastic hard-sphere model is used, and in the event driven approach the particles follow an undisturbed Newtonian motion, under the influence of gravity, until an event occurs. An event is either the collision of two particles or the collision of one particle with the wall. The time during which two particles are in contact is implicitly zero. The hard-particle collision model uses momentum conservation laws and the definition of the coefficient of normal and tangential restitution to determine the states of particles after a collision.

Parallel Analog and Logic Electronic Simulation System (PALESS) presents Gridenabled simulation of modern electronic circuits and systems which are very complex (tens of millions of transistors), and can be applied in complex surroundings including sensors, actuators and other devices not directly connected to electronics, but whose behavior can be described in a different non-electrical natural domain (such as mechanical, chemical, biological etc.).

The proper elements of asteroids are used to classify asteroids into families, and to study the dynamical and collisional evolution of the asteroid belt, and of the Solar system as a whole. Their calculation is made possible in an efficient way by the gridified version of **Asteroid Proper Elements Calculation (PROPEL)** application. This application in the Grid environment presents a powerful tool to study the problems of the stability of motion, resonant and chaotic phenomena.

Grid-based Visual interactive general purpose discreet event simulator - **SLEEP** - simulates digital circuits made in VLSI technique for educational purposes and verification of business process integration. Simulator is able to use set of independent basic elements connected with single target simulation. The appropriate tools implemented within this simulator should be able to help end users to write their own simulators easier.

5. Grid training activities

The training activities are seen as one of the crucial tasks within AEGIS community, as well as by EGEE-III and SEE-GRID-SCI project. Such activities are effective way of introducing new users to the world of Grid. At the same time, even the experiences users are regularly informed about new developments and improvements in Grid technology, in available computing and storage resources, and also in available software environments and libraries in the national, regional and pan-European eInfrastructures. The organized training events serve two purposes: to develop and validate the shared pool of best practices, training materials and resources, and to initiate direct contact of users, developers and system administrators.

The Grid training courses are mainly organized by SCL at the national and regional level in Serbia, with strong participation and support in co-organizing training events in other countries in the region. The courses cover a wide range of competences and skills from induction-level courses focusing on newcomers to Grid computing, to more advanced courses aimed at application developers working on porting of their applications to the Grid. Many courses are also designed for site administrators responsible to operate Grid sites.

6. Conclusions

AEGIS Grid eInfrastructure provides more than 1000 CPUs and 30 TB of data storage to all user communities through a distributed set of Grid sites hosted by major research institutes and universities. This eInfrastructure is fully utilized by a number of scientific highperformance applications, developed Serbian researchers and adapted for optimal use on the Grid with the support of the Scientific Computing Laboratory of the Institute of Physics Belgrade. Such support is provided either directly for specific applications, or through advanced training activities for application developers. Serbia has long-standing strong participation in European Grid projects and has established a reliable and extensive national Grid eInfrastructure, which provides advanced computing services not only to national research community, but also to other researchers from user communities supported by EGEE and SEE-GRID programmes. The AEGIS eInfrastructure also stimulated further collaboration of Serbian and European researchers, and helped in bringing the issue of providing support for research infrastructure to the agenda of Serbian policy makers. For these reasons, AEGIS also actively participates and works with other NGIs on establishing a sustainable European Grid Initiative, which should provide stable environment for scientific communities with high-performance computing requirements.

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