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ACCESS TO THE REGIONAL SCIENTIFIC COMPUTING INFRASTRUCTURE

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Scientific Computing Infrastructure and related technologies developing for Eastern Europe's Research Communities will link existing and upcoming computational facilities in the region in a common infrastructure that has perspective to be integrated in top-level European computational eInfrastructure, and it will provide access to modern computational resources to wide range of researchers and attract new research communities. Realization of a serious of regional eInfrastructure projects allowing regional research communities to get access to the computing resources of leadership-class capability and will remain competitive at the European and international level, thus overcoming fragmentation in European regions development.

Introduction

The transition of the traditional science to e-Science is fueled by the ever increasing need for processing of exceedingly large amounts of data and exponentially increasing computational requirements: in order to realistically describe and solve real-world problems, numerical simulations are becoming more detailed, experimental sciences use more complicated instruments to make precise measurements; and shift from the individuals-based science work towards collaborative research model now starts to dominate. In this context the role of scientific computing that comprises Grid, High Performance Computing (HPC) and intensively developing scientific clouds in the modern research is crucially increasing. It considerably determines the level of development of the knowledge based society. Mathematical modeling forms a solid theoretical and applied basis in describing, simulating and studying the complex problems. The regional and European cooperation in the field of scientific computing represents an important factor for developing of the research activities and determine perspectives of integration the in the European Research Area.

Although in the past years the European Commission has funded, through a number of targeted initiatives, creation of new user communities and enabling collaborative research across a number of fields. In Eastern Europe the eIfrastructure in the region in general is less developed than in Western Europe [1]. Advancing the Information Society in areas such as South-East Europe, strengthening of the local eInfrastructures, activating new user communities and enabling collaborative research across a number of fields, would strongly contribute to closing the existing technological and scientific gap, and thus bridging the digital divide, stimulating research and consequently alleviating the brain drain in the region.

1. National and regional strategies of scientific computing technologies development

Historically in Moldova the first scientific computing resources had begun developing from the initial deployment in 2006 of the first Grid cluster that was integrated in the regional South-Europe Grid infrastructure. This specific and new for Moldova activities were supported by a range of the SEE-GRID projects [2,3]. These projects have allowed establishing of strong human network in the area of scientific computing and have set up a powerful re-

gional Grid infrastructure. This is very much in line with the European vision of moving towards a long-term sustainable European Grid Initiative through strong support of National Grid Initiatives (NGI), and, in this aspect, SEE-GRID is to some extent leading the way by its successful establishment of NGIs in the region, including Moldova. One of main objectives of the SEE-GRID projects was to penetrate and engage regional and national user communities via multi-disciplinary grids, involving a range of research and academic institutes and scientific communities in all SEE countries, with emphasis on the deployment and support of a range of Grid applications. This first experience was successful from the point of view of forming professional team of specialists in the area of distributed computing and initiated the process of examination needs of potential users' teams in computational resources that pave the way for creation in future of prepared national users community. Main directions of the created in 2007 National Grid Initiative can be summarized as following:

- MD-Grid NGI participates in strategic European Programs for the development of transnational grids and in initiatives for the completion of SEE eInfrastructures. The operation of the MD-Grid NGI implements the general EU policy on the development of national initiatives for the coordination of actions related to eInfrastructures and especially to scientific computing infrastructures.
- The integration of Grid actions (infrastructures, middleware and applications) with the broadband research and technology network into a standard e-Infrastructures system. Optimization of exploitation of advanced network resources and services, which can serve the new e-Science generation and will attract the greater users' community of the Information Society to the mass adoption of advanced services provided by Grid architectures.
- Permanent development and administration of Grid infrastructure in Moldova.
- Organization access for national users' community to the regional and European computational resources (HPC, Grid, scientific clouds, etc.).
- Preparing (educational and training events organization) and support of national users' communities.

One of main NGI activities is permanent development of Grid infrastructure in Moldova. Now Grid infrastructure unites three sites and has well determined perspectives for its further enlargement. Another principal task that is in focus of NGI is monitoring of research and educational community needs and attracting new research teams that have requirements in complex applications development and in access to special computing resources. Contacts with members of the community and analysis of their needs had shown that there are special needs in computational resources that can't be covered only by Grid infrastructure. That's why MD-Grid NGI argued necessity, supported initiation and actively participating in new regional scientific computing activities development like HPC and cloud computing.

In the field of High Performance Computing the European Commission supports a series of initiatives to provide access to HPC facilities to leading European Researchers. The SEE region is still lagging behind the European developments in the HPC area. Only few HPC installations are available – one large supercomputing top500 installation in Bulgaria and some smaller HPC ones in couple of other countries, and these are not open to cross-border research. The user communities using HPC are limited. Similarly, the less-resources countries have no established mechanism for interfacing to European HPC infrastructures like PRACE, DEISA, or any other related initiatives. Thus, regional eInfrastructure must be expanded to address these specific needs of scientific and engineering communities in the region. Furthermore the region has a strong need to acquire and maintain expertise in the provision and utilization of HPC facilities both at the system as well as the software level.

To cover the permanently rising needs of research communities in the SEE region there was elaborated and proposed for funding regional eInfrastructure development project -"High-Performance Computing Infrastructure for South East Europe's Research Communities (HP-SEE)". The HP-SEE project (http://www.hp-see.eu/) started in September 2010 and brings together 14 partners from the SEE region, while more than 10 institutions have been involved in the project as third parties. Less-resourced countries like Moldova have no mechanism established for interfacing to pan-European HPC initiatives. South-East European HPC initiative is aimed for equal participation of all countries of the region in European eInfrastructure development trends. HP-SEE focuses on a number of strategic actions [4]:

First, it will link existing and upcoming HPC facilities in the region in a common infrastructure, and provide operational solutions for it.

Second, it will open this HPC infrastructure to a wide range of new user communities, including those of less-resourced countries, fostering collaboration and providing advanced capabilities to researchers, with an emphasis on strategic groups in computational physics, chemistry and life sciences.

Finally, it will ensure establishment of national HPC initiatives. HP-SEE will aim to attract local political & financial support for long-term sustainable eInfrastructure.

Development of scientific clouds is rather new, but perspective direction of computational technologies development. For SEE region needs in cloud technologies deployment were analyzed during execution of SEERA-EI project funded by EC ERA-NET Programme. The analysis produced had shown strong interest of the regional research communities in scientific clouds technologies deployment. In many countries this perspective direction is supported by governmental strategies as new technological approach for providing wide range of e-governmental services. As a resulting outcome of SEERA-EI project was recommendation to launch regional Pilot Call for projects in the area of scientific cloud computing. This Call was recently announced (http://www.seera-ei-pjc.asm.md/) and one of its priority topics is feasibility study of approached for scientific clouds integration to the announced e-government cloud infrastructures in the region.

2. Access possibilities to the HP-SEE computing resources

Regional scientific computing infrastructure development is coordinating with pan-European initiatives like EGI-InSPIRE project that is focused on supporting transition process from a project-based system (the EGEE series) to a sustainable pan-European e-Infrastructure. EGI-InSPIRE activities are covering grids of high-performance computing (HPC) and high-throughput computing (HTC) resources. The project integrates new Distributed Computing Infrastructures (DCIs) such as clouds, supercomputing networks and desktop grids, to benefit the user communities within the whole European Research Area.

In the project there two categories of partners – partners that have their own HPC recourses, co called "resource providers" and partners - beneficiaries. Beneficiary countries like Moldova are receiving preferences from gaining access to resources that are provided by other project partners in the region - "resource providers".

From Moldova in the project involved MD-GRID NGI represented by its coordinator - RENAM Association (National Research and Educational Network of Moldova) and Institute of Mathematics and Computer Science of the Academy of Sciences of Moldova (IMI ASM). MD-GRID NGI efforts are emphasized on the involvement of national communities to the use of regional infrastructure for high performance computing, training activities and applications operational support. IMI ASM main task is the development of HPC applications and deploying them in regional HPC infrastructure.

The Regional HPC infrastructure integrates the most powerful HPC clusters and supercomputers provided by the main infrastructure partners from the 6 countries, participating in the project: Greece - Greek Research & Technology Network; Bulgaria - Institute of Information and Communication Technologies (IICT), Bulgarian Academy of Sciences; Romania - "Horia Hulubei" National Institute of Research and Development for Physics and Nuclear Engineering; Hungary - National Information Infrastructure Development Office; Serbia - Institute of Physics, Belgrade; FYROM (Macedonia) – SS Cyril & Methodius University of Skopje.

The structure of the regional HPC infrastructure is heterogeneous, comprising supercomputers, Intel/AMD CPU and GPU clusters. HPC resources available for user' community include Blue Gene/P supercomputer deployed at Executive Agency "Electronic Communications Networks and Information Systems" in the Bulgarian Supercomputing Centre (BGSC), consisting of two racks, 2048 PowerPC 450 based compute nodes, 8192 processor cores and a total of 4 TB random access memory. Supported parallel programming paradigms are MPI and OpenMP. There is also possibility to run jobs in HTC mode (High Throughput Computing).

Main resources of the regional HPC infrastructure support parallel programming paradigms like MPI and OpenMP. Most of them also offer possibility to run jobs in HTC mode (High Throughput Computing).

Table 1. HP-SEE Infrastructure current status and plan of development

Country	**TFlops**			
	2010	**2011**	**2012**	**2013**
Greece	0	0	40	80
Bulgaria	25	31+8GPU	31+20GPU	40+20GPU
Romania	10	26+4GPU	30+20GPU	30+20GPU
Hungary	1	48	48+12GPU	48+12GPU
Serbia	6	6	20	20
OVERALL	**42**	**111+12GPU**	**169+52GPU**	**218+52GPU**

Partners participating in the HP-SEE project have established HPC training infrastructure as the necessary prerequisite for the successful organization of various training events. Also this infrastructure can be used for applications elaboration, testing and debugging. During the project execution there was produced upgrade of the existing training infrastructure in Moldova. IMI-RENAM Grid cluster (8 servers) was fully transferred to the virtualization platforms. The resources of this cluster are permanently developing to fit the needs of domestic applications development, testing and debugging. For this purpose it was made additional reconfiguration of Windows Compute Cluster (WCC) 2003 software: WCC was entirely transferred on the virtualization platform; current WCC 2003 Cluster configuration is up to 20 cores on 6 servers, max 8 cores per one Virtual Machine [5].

All applications that are developing in the project are grouped within the three Virtual Research Communities (VRC): Computational Physics (CP), Computational Chemistry and Life Sciences Virtual Research Community.

Among CP applications adapting on the regional HPC is AMR_PAR application (Parallel algorithm and program for the solving of continuum mechanics equations using Adaptive Mesh Refinement), developed in the Institute of Mathematics and Computer Science of the

Academy of Sciences of Moldova. In the AMR_PAR application is considering a continuum mechanics problem, such as the problem of modeling the explosion of a supernova type II and, for this example, created an algorithm using the method of AMR and construction of the parallel program [5].

This method can be applied to any other nowadays problem of continuum mechanics - to calculate the aerodynamics of aircraft, the calculations of the air flow of cars, a large number of other problems of mathematical modeling - calculation of the flow of blood through the vessels, the calculations of the heart valves, etc. Hence, the practical use – the calculation of complex problems in a reasonable time. In all these cases, at the beginning of the problem we define a way to highlight areas in which need to construct the grid, then the program builds a sequence of grids and makes a decision on them. The social impact depends on the problem to be solved, the use of AMR_PAR being of interest for heavy industry (e.g. car body design and development, aircraft aerodynamics), or for healthcare industry.

For every application developing in the project are assigned at least two specific computational recourses (home clusters) available in the regional HPC infrastructure. The home clusters for AMR_PAR application are the SGI UltraViolet 1000 supercomputer at the National Information Infrastructure Development Institute (NIIFI), located in Pecs, Hungary (1152 CPU, 6057 GByte of memory) and HPCG cluster, located at the Institute of Information and Communication Technologies of the Bulgarian Academy of Sciences (576 computing cores; the storage and management nodes have 128 cores).

4. Conclusion

Permanent developing of scientific computing facilities aspires to contribute to stabilization and development of research and Hi-Tech activities in Eastern Europe, by overcoming fragmentation in Europe and stimulating eInfrastructure development and adoption by new virtual research communities, thus enabling collaborative high-quality research across a spectrum of scientific fields.

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