Access to the Regional Scientific Computing Infrastructure for Research Community of Moldova

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Abstract. *Scientific Computing Infrastructure, related technologies and services have begun developing for R&D communities of Moldova due to the support of a series of international and national projects. Project HP-SEE - High-Performance Computing Infrastructure for South East Europe's Research Communities will link existing and upcoming HPC facilities in South East Europe in a common infrastructure, and it will provide access to HPC resources to wide range of researchers. It will provide access to modern computational resources to wide range of researchers, attract new research communities in Moldova and promote joint research activities at national, regional and European levels. The realization of eInfrastructure development projects will allow national 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.*

Keywords

Scientific Computing Infrastructure, eInfrastructure, HPC, High-Performance Computing, Balanced Regional Development

1 Introduction

The transition of the traditional science to e-Science is fueled by the ever-increasing need for processing 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. Now the shift from the individuals-based science work towards collaborative research model starts to dominate.

In this context the role of Scientific Computing (HPC, Grids, Cloud computing) in the modern scientific research is crucially increasing. It considerably determines the level of development of the scientific knowledge based society. Mathematical modeling forms a solid theoretical and applied basis in describing, simulating and studying the complex problems. The international cooperation in the field of Scientific Computing represents an important factor for developing the area of scientific research and perspectives of the European future for research community of Moldova.

In the last years Moldova as a part of South-East Europe (SEE) actively participated in a number of targeted initiatives funded by the European Commission, focused on the creation of new user communities, and enabling collaborative research across some fields in South-East Europe. Although the necessary initial contributions in the region were done, the computational facilities available now are in general less developed than in Western Europe [1].

Advancing the Information Society in such countries as Moldova, strengthening 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 and consequently alleviating the brain drain in the region of South-East Europe.

2 Access to the regional HPC resources and strategy of their development

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.

To cover the permanently rising needs of researchers in SEE region the regional eInfrastructure development project "High-Performance Computing Infrastructure for South East Europe's Research Communities (HP-SEE)" was elaborated and proposed for funding. 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 research institutions have been involved in the project as third parties. The project has begun with only few HPC installations available, being not open to cross-border research. The aim of the South-East Europe HPC initiative is the equal participation of all countries of the region in European eInfrastructure development trends.

HP-SEE focuses on a number of strategic actions [2]:

First, it will link the existing and upcoming HPC facilities in the region in a common infrastructure, and will 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 the collaboration and providing advanced capabilities to researchers, with an emphasis on strategic groups in computational physics, chemistry and life sciences.

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

RENAM Association (National Research and Educational Network of Moldova) and the Institute of Mathematics and Computer Science of the Academy of Sciences of Moldova (IMI ASM) are involved in the project from Moldova. RENAM efforts are emphasized on the promotion of national communities to the use of the regional infrastructure for high performance computing, training activities, applications porting and operational support. The main task of IMI ASM is the development of HPC applications and the deployment of them in the regional HPC infrastructure [3].

In the project there are two categories of partners, which form the project consortium – partners that have there own HPC recourses, so called "resource providers" and partners - beneficiaries. Beneficiary countries like Moldova receive preferences from gaining access to resources available in the other project partners in the region - "resource providers".

The regional HPC infrastructure integrates the most powerful HPC clusters and supercomputers provided by the main infrastructure partners from the six countries, participating in the project: Greece, Bulgaria, Romania, Hungary, Serbia, and FYROM (Macedonia) – see table 1.

Tab.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

The structure of the regional HPC infrastructure is heterogeneous, comprising supercomputers, Intel/AMD CPU and GPU clusters. HPC resources available for users' community from Moldova 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.

There is also possibility to run jobs in HTC mode (High Throughput Computing). Another resource is the HPCG cluster located in IICT of the Bulgarian Academy of Sciences. It has 576 computing cores organized in a blade system. The storage and management nodes have 128 cores. There is an agreement with the West University of Timisoara (Romania) concerning access of Moldavian researchers to the Blue Gene/P supercomputer, the installation of which has been finished recently.

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 High-Throughput Computing (HTC) mode.

3 AMR_PAR application (parallel algorithm and program for solving continuum mechanics equations using Adaptive Mesh Refinement)

All applications that are developing in the project 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 infrastructure there is AMR_PAR application (parallel algorithm and program for solving continuum mechanics equations using Adaptive Mesh Refinement), developed in the Institute of Mathematics and Computer Science of the Academy of Sciences of Moldova.

The AMR_PAR application is considering a continuum mechanics problem, and namely the problem of modeling the explosion of a supernova type II and, for this example, created the algorithm and parallel program using the AMR method [4,5].

Calculations method based on the use of AMR hierarchical grid cells can significantly improve the quality of the calculations in the various fields of science and engineering calculations. In addition, the most of applications that using AMR is well parallelized on supercomputers. We use the programming language Fortran 90. Program based on AMR technology uses object-oriented approach, which is available in Fortran 90 [6].

The first version of the application was developed using MS Visual Studio 2010 (for OS MS Windows) on a PC with a processor Intel Core I7 920, 2.667 GHz. Calculations were performed using option “collapse”, and without it. Option “collapse” is used for apportionment of the iterations in strongly nested loops. In figure 1 is a graph of the acceleration depending on the number of processor cores for computational grid 128x128x128. The graph with triangles shows acceleration achieved using options “collapse’ on three nested loops, graphs with circles shows acceleration with “collapse” on 2 cycles and squares shows acceleration without “collapse”.

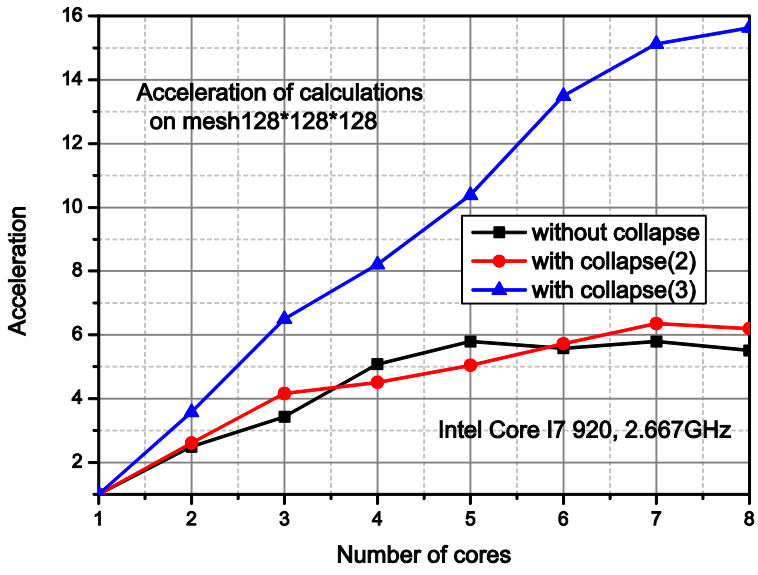

Fig.1 Intel Core I7 920, acceleration for computational grid 128x128x128

Note that the use of this directive for three strongly nested loops greatly speeds up the program. This is because for all cycles a common space of iterations is formed, which is divide between all threads.

The AMP_PAR application testing performed initially in OpenMP mode on Microsoft Windows Compute Cluster 2003 in the Institute of Mathematics and Computer Science of the Academy of Science of Moldova. The benchmarking results of MS Windows version of the application summarized and presented on figure 2 (WCC2003 computer nodes equipped with 2 x QuadCore Intel Xeon E5310, 1600 MHz, 8 GB of RAM).

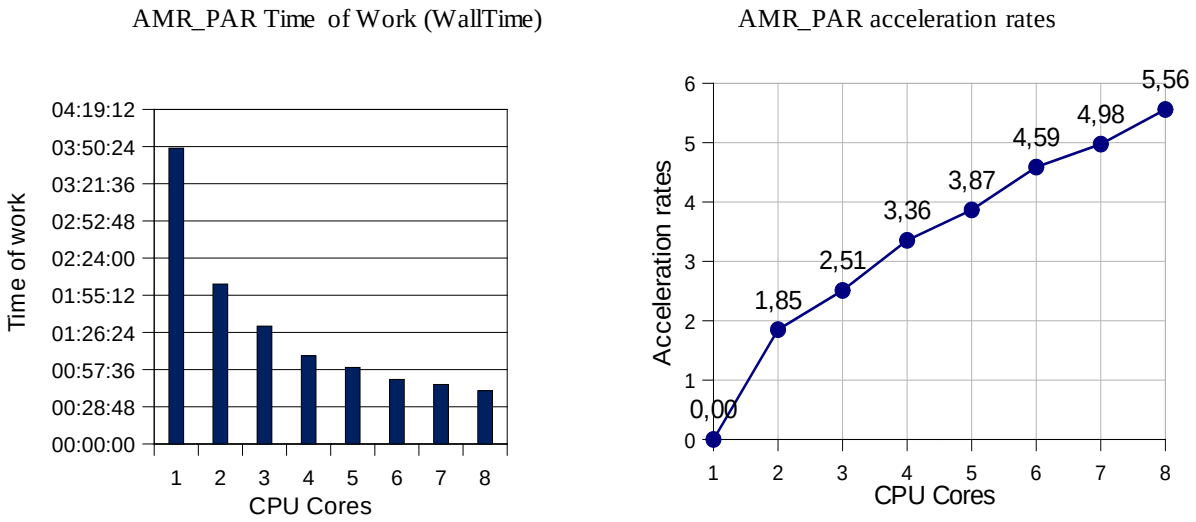

Fig.2 Intel Xeon E5310, acceleration for computational grid 128x128x128, MS Windows

Then AMR_PAR application was prepared for running using regional HPC resources provided by HP-SEE project. Application in OpenMP mode was compiled on virtual machine with Linux and Intel® Parallel Studio XE 2011 for Linux. The results obtained during the tests had shown existing of the problem of the application scalability. On the base of the tests' results AMR_PAR application was modified in order to work with large-scale grids' dimensions. Modified version of AMR_PAR application passed scalability tests on local resources - Virtual Machine – up to 8 Cores, RAM up to 24 Gb.

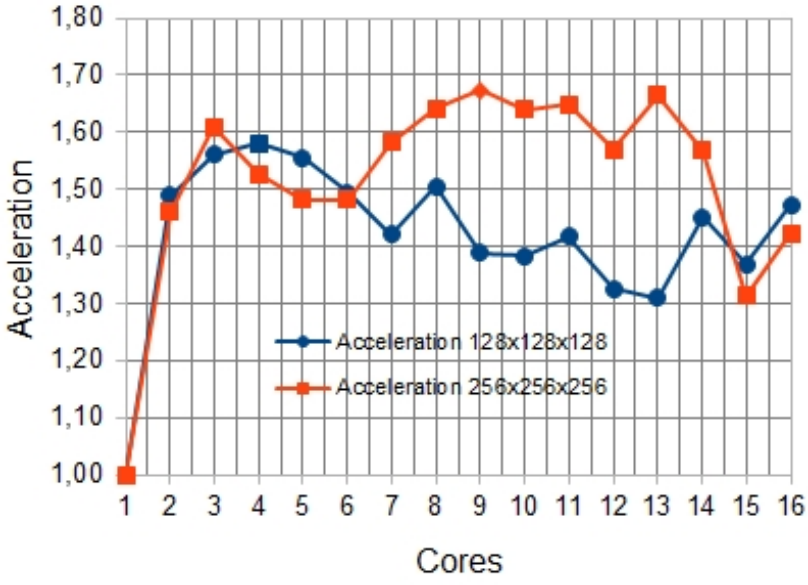

Fig.3 Acceleration dependences from number of CPU cores (HPCG cluster, Linux)

Next tests were performed on HPCG cluster located at the Institute of Information and Communication Technologies of Bulgarian Academy of Sciences (Linux, each node has 2 Intel XeonX5560, 2,8 Ghz, 24 Gb RAM). Benchmarking results were collected for the following dimensions: 128x128x128, 256x256x256. For arrays of

128x128x128 dimension with five levels of nesting optimal number of cores for calculation is about 4. Otherwise, the increasing of number of cores is not reducing of wall-clock time of calculations, but processing time increases dramatically (see figure 3). It should be noted a drop of acceleration in comparison to the previous calculations.

4 Achieved Results and Foreseen Activities

After calculation of the necessary amount of RAM for grid dimensions up to 2048x2048x2048 cells, as home cluster for the application porting was proposed the SGI UltraViolet 1000 supercomputer at the National Information Infrastructure Development Institute, located in Pecs City, Hungary (SMP, 1152 cores and 6057 GB RAM). For small grids (up to 384x384x384 cells) resources of HPCG can be used.

Tab.2. Benchmark results and forecasting demands for resources

Dimension	Layers	Max Iteration per level	Cores	RAM Gb	CPU time	WallTime
128x128x128	5	200000	4	0,789	28 min	3,5 min
256x256x256	5	200000	8	6,062	527 min	66 min
384x384x384	5	200000	8	19,2	2110 min	270 min
448x448x448	5	200000	8 — 16	37,7	~ 4500 min	~ 500 min
512x512x512	5	200000	8 — 16	~ 55,6	~ 130 hours	~ 17 hours
1024x1024x1024	5	200000	16 — 32	~ 415	~ 2000 hours	~ 248 hours
2048x2048x2048	5	200000	32 — 64	~ 3250	~ 1200 days	~ 154 days

For further optimization of AMR_PAR application, we plan collecting statistics of calculations' acceleration dependences from different number of cores - up to 32 (or more). It is necessary to produce investigations to find optimal number of cores for fastest calculations for large-scale grid dimensions. As a result of this research we plan to modify the application to use OpenMP more effectively.

Next step is to run application using HP-SEE regional resources for large-scale grid dimensions – up to 2048x2048x2048 and 5-7 layers. For this purpose the application was adopted to run on SGI UltraViolet 1000 supercomputer at the National Information Infrastructure Development Institute, located in Pecs City, Hungary (SMP, 1152 cores and 6057 GB RAM). After obtaining results of the modified application execution, it will be possible to make new benchmarking (due to long time of forecast calculations) and propose new recommendations for application optimization. Updated application also will allow describing and visualization of results in a form of 2-D images and 3-D models.

5 Applying of experience gained in the HP-SEE project

For developers and users of complex applications from the beneficiary countries of South-East Europe within framework of the signed Agreement "Memorandum of Understanding for High-Performance Computing resource sharing in the region of South Eastern Europe" are accessible high capacity computer resources of more than 10 HPC regional installations. These resources are available for the members of the project staff and also for users and parallel applications developers from others scientific and educational institutions of Moldova and other participating in the project countries.

Experience, obtained in the HP-SEE project allowed to elaborate and propose for funding new project "Instrumental support for complex applications porting to the regional HPC infrastructure". New consortium was formed for this project that brings together the following organizations:

- Moldova State University of Ministry of Education of Moldova;
- Institute of Mathematics and Computer Science of Academy of Sciences of Moldova;
- Public Association RENAM (supervised by the Academy of Sciences of Moldova and the Ministry of Education).

The new project is supported by international funding organization - Science & Technology Center in Ukraine (STCU). Aims of the project are to provide analysis for development, adaptation and porting to the available regional HPC infrastructure scalable applications for solving problems that require significant computational resources. As practical tasks for applications development are considering the problems of such areas as computer added design of semiconductor devices and decision-making modeling.

Solution of the semiconductor devices modeling task with acceptable accuracy is requiring enormous computational resources. For designing of semiconductor devices will be used the model of drift-diffusion approximation, which leads to the necessity of constructing efficient algorithms for solving systems of nonlinear differential equations with partial derivatives on multiprocessor systems.

For solving the decision-making problems will be used algorithms based on game theory. The project proposes to develop and implement parallel algorithms for solving the decision-making problems using the theory of advanced informational games and realize experimental simulation on HPC systems. The developed models can be used as a basis for analyzing decision-making processes in situations of risk and conflicts assessment in different economical systems, as well as in other areas of practical interest. The proposed implementation can be used in variety of parallel systems such as clusters and in distributed computing systems.

In order to develop applications, training of users and software developers will be used computational resources of two existing and rather small local clusters in the Institute of Mathematics and Computer Science and in the State University of Moldova. For these systems will be specified and installed toolkits necessary for the elaboration of complex applications, will be completed the unification of software environments and created interfaces to share the resources of both clusters for developing and running applications.

Elaborated and tested on the local infrastructure applications will be proposed for porting and production execution in the regional HPC infrastructure, available to research and educational users' community of Moldova as part of the HP-SEE project activities.

6 Acknowledgements

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