Computational Infrastructure for Porting and Execution Complex Applications in Moldova

Bogatencov P., Iliuha N.
RENAM Association,
Chisinau, Moldova,
bogatencov@renam.md

Calmis E., Hancu B., Patiuc V.
State University of Moldova
Chisinau, Moldova,
boris.hancu@gmail.com

Secrieru G.
Institute of Mathematics and Computer Science of ASM
Chisinau, Moldova,
secrieru@cc.acad.md

***Abstract* — This paper presents the experience of creation and operation of the computing infrastructure that incorporates the resources of multiprocessor clusters of the State University of Moldova and the Institute of Mathematics and Computer Science of ASM with access to European computing infrastructure for the development, implementation and porting complex parallel application. The main results are obtained during the realization of the international project "Instrumental support for complex applications porting to the regional HPC infrastructure" supported by the Science and Technology Center in Ukraine (STCU).**

***Keywords* — HPC, Cloud, Grid computing, regional e-Infrastructures, parallel algorithms and applications**

I. Introduction

In recent years we see the rapid development of distributed information processing and high-performance computing (HPC installations, distributed Cloud and Grid computing infrastructures) technologies for solving complex tasks with high demands of computing resources. In Moldova the works on creation of high-performance and distributed computing infrastructures were started relatively recently due to participation in implementation of a number of international projects. Moldovan scientists actively participated in the regional and pan-European projects, including initiatives focused on integration in pan-European e-Infrastructures. That allowed research teams from Moldova to get access to national, regional and European computing resources and expand the range and areas of complex mathematical modeling tasks.

II. Current State of the Computing Infrastructure in Moldova

A. HPC infrastructure development

European institutions are paying significant attention to new initiatives for the development of high-performance computing infrastructures, resources and technologies to support development and execution of complex parallel applications. In recent years, several initiatives have been launched, aimed at creating of supercomputer centers and their integration into a common European HPC infrastructure. Since mid of 2000' Moldova is actively involved in regional and European programs for cooperation in the field of scientific computing. Taking into account the significant investments in creating of high-performance computing infrastructures in Europe, currently main attention is focused on designing and implementation of instrumental support for rising effectiveness of unique computing systems. Coordination of activities in this area is carried out within the European initiatives like PRACE project (Partnership for advance computing in Europe) that has the aim to create a common HPC ecosystem. This ecosystem has to bring together providers of computing resources and diverse users' communities - from research, educational institutions and specialized software companies as well as from small, medium and large enterprises - consumers of computational experiments results. HPC ecosystem includes several levels of HPC installations depending on their performance and directions of use. On the top "zero" level (Tier-0) supercomputing resources of the world leading supercomputer centers are located. HPC facilities available in Moldova (taking into account their real capacity) at present correspond to Tier-2 level representing HPC centers of research institutes and universities [1].

In 2004-2006, due to realization of the project supported by CRDF-MRDA at the State University of Moldova, the first computing cluster with parallel architecture was installed. Initially, the cluster has the following specifications: 4 Servers HP ProLiant DL385G1 (CPU: AMD 280 Dual-Core 2.4GHz, RAM: 2GB Reg. PC3200 DDR, HDD: SmartArray 6i, 2x146GB 10k, Network: 3x1Gbps LAN); 12 knots HP ProLiant DL145R02 (CPU: 2xAMD 275 Dual-Core 2.2GHz RAM: 4GB AECC PC3200 DDR HDD: 80GB NHP SATA Network: 3x1Gbps LAN); disk system HP SmartArray 6402 (Enclosure: hp StorageWorks MSA20, HDD: 4x500GB 7.2k SATA). The cluster configuration is permanently upgraded.

The second computing complex with parallel architecture was jointly created by the Institute of Mathematics and

Computer Science of ASM and RENAM Association. The parallel cluster installed in 2007 includes 8 servers with the following parameters: 48 cores Xeon E5310, E5335; 64 Gb RAM; 3,6 Tbyte HDD. This computing system was created due to support of the European SEE-GRID regional projects and bilateral co-operation project funded jointly by ASM and Russian Foundation for Fundamental Research.

Important for Moldova was participation in the regional project HP-SEE (High-Performance Computing Infrastructure for South East Europe's Research Communities) that allowed for local research and educational institutions to get access to regional HPC resources [2]. Regional HPC infrastructure combines powerful HPC clusters and various supercomputers provided by the project participants from five countries involved in the project: Greece, Bulgaria, Romania, Hungary and Serbia. Regional HPC infrastructure is heterogeneous - includes supercomputers and clusters based on Intel/AMD CPU and GPU. HPC resources that are offering to users' community included also two supercomputers IBM Blue Gene/P installed in the Bulgarian Supercomputing Center of the Agency "Electronic Communication Networks and Information Systems" and in the Western University of Timisoara (Romania).

During HP-SEE project realization in Moldova have been identified and proposed for implementation several technologies and tools for offering access to advanced computing resources and services that developing for researchers from South-Eastern Europe, including from Moldova. Members of the project from Moldova participated in a series of specialized trainings organized within HP-SEE, LinkSCEEM-2 and PRACE projects. For providing access for developers and users of complex applications from scientific and educational institutions of Moldova in the framework of HP-SEE project in 2012 was signed the Cooperation Agreement between RENAM and computer centers in South-Eastern Europe. The Agreement determines conditions of providing access to the regional high performance computing resources that comprises more than ten high-performance systems.

HP-SEE project achieved its aim to strengthen scientific cooperation and to promote activities in the field of high performance computing. As a result, it contributed to regional development and involvement of Moldova into the European HPC resources development trends [3].

The STCU funded project "Instrumental support for complex applications porting to the regional HPC infrastructure" allowed continuing of the national computing infrastructure development activities. The project aim was analysis, adaptation, development and porting to the national and regional high-performance computing infrastructures of scalable applications for solving tasks that need large volume of computational resources [4].

The project activities comprised construction of efficient parallel algorithms and elaboration of the appropriate software for solving problems of computer aided design, modeling of semiconductor devices on multiprocessor systems. For practical development of parallel application for solving tasks of computer aided design of semiconductor devices as one of the of the project objectives was creation of a specialized run time environment that included the use of PETs open source software package for solving nonlinear differential equations systems in partial derivatives. For the design of semiconductor devices diffusion-drift approximation is used, which leads to the necessity of solving a high dimension system of nonlinear differential equations in partial derivatives.

The second task developed within the project was elaboration of parallel algorithms for solving informational expanded games. The parallel application elaborated for this task is using the open source ScaLAPACK software package for solving models of linear systems. The elaborated application is using also MPI and OpenMP standardized functions for this parallel application execution on computer systems with common and distributed memory.

Within the STCU project was elaborated specialized software environment and developed programming tools for uniting the individual cluster's systems of the Institute of Mathematics and Computer Science of the Academy of Sciences of Moldova and the State University of Moldova in the integrated distributed parallel computing system. This allowed porting of the developed applications that are realizing the proposed parallel algorithms on this integrated system for their debugging, testing and performance optimization.

B. Distributed computing infrastructure development

Distributed computing infrastructures and services are very important component of the modern scientific-educational e-Infrastructures. Historically the first distributed computing infrastructure deployed in Moldova was Grid computing infrastructure - a specific e-Infrastructure element, which provides remote access to distributed computing power. Grid infrastructure is able to offer:

- Joint use of computing resources
- Access to distributed data storage resources
- Shared access to large experimental facilities and remotely controlled experiments
- Creating a distributed experimental facilities and resources
- Automatic retrieval of data and resources in the network
- Promoting cooperation and joint implementation of projects.

The scientific computing resources in Moldova had begun developing from the initial deployment in 2006 of the first Grid cluster that was integrated in the regional South-East Europe Grid infrastructure. These specific and new for Moldova activities were supported by a serious of the regiona SEE-GRID projects [5]. These projects allowed establishing strong human network in the area of scientific computing and set up a powerful regional 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). SEE-GRID projects leaded the activities of successful establishment of NGIs in the region, including in 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 wide range of Grid applications. RENAM Association, representing national scientific-educational network of Moldova (NREN), started to build MD-Grid NGI in 2006. National Grid Initiative of Moldova represented by the Joint Research Consortium was created within the framework of the European Commission SEE-GRID-2 project [6]. MD-Grid NGI was inaugurated on May 14, 2007 after receiving approval letters from Ministry of Information Development of Moldova and the Academy of Sciences of Moldova. The MD-Grid NGI Consortium is governed by RENAM as its Coordinating body and joins nine research, education institutions and industry that expressed their intent to participate in the processes of building National Grid Infrastructure and using its resources. The major steps in the establishment of MD-Grid NGI included:

- the development and approval of MD-Grid NGI Foundation document (Consortium Agreement),
- the development and approval of MD-Grid NGI Policy document,
- the negotiation with potential MD-Grid NGI members conditions of their participation in the NGI,
- signing the agreements (MoUs) with MD-Grid NGI potential members,
- planning the Grid infrastructure enlargement, creation and setting up at the beginning stage at least three Grid-sites in research and higher educational institutions of Moldova.

The elaborated MD-Grid NGI Policy document stipulates basic principles of NGI Consortium behavior and requirements for NGI supported services:

- NGI membership rules. NGI member organizations should belong to four main categories: research, academia, industry and government.
- Accessible Use Policies and Services Level Agreements for resources and services.
- National Grid Certification (Registration) Authority policy and behavior.
- Core services structure and functions.

The initially accumulated experience was successful from the point of view of forming professional team of specialists in the area of distributed computing and examination of potential users' communities needs in computational resources that pave the way for creation of the prepared national users' community in future. The main activity directions of the created in Moldova National Grid Initiative are summarized as following:

- MD-Grid NGI participates in strategic European Programs for the development of transnational distributed computing technologies and in initiatives for the completion of regional e-Infrastructures. 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 e-Infrastructures and especially to scientific computing infrastructures.
- The integration of distributed computing development actions (infrastructures, middleware and applications) with the broadband network into a standard e-Infrastructures system. The 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 modern computing architectures.
- The permanent development and administration of the computing infrastructure.
- The organization access for national users' communities to the regional and European computational resources (HPC, Grid, scientific clouds, etc.).
- The educational and training events organization; the technological and consultancy support of national users' communities.

NGI is engaged in the development of Grid infrastructure in Moldova. At present Grid infrastructure unites three sites (see Fig. 1) and has well determined perspectives for its further enlargement. Another principal task that is in focus of NGI is monitoring the research and educational community needs and attracting new research teams that have requirements in complex applications development and in access to special computing resources [7].

The development of national and regional scientific Grid infrastructures since 2010 is coordinating by pan-European initiatives like EGI-InSPIRE project that focused on supporting transition process from a project-based system (the EGEE series) to a sustainable pan-European e-Infrastructure. EGI-InSPIRE activities cover 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.

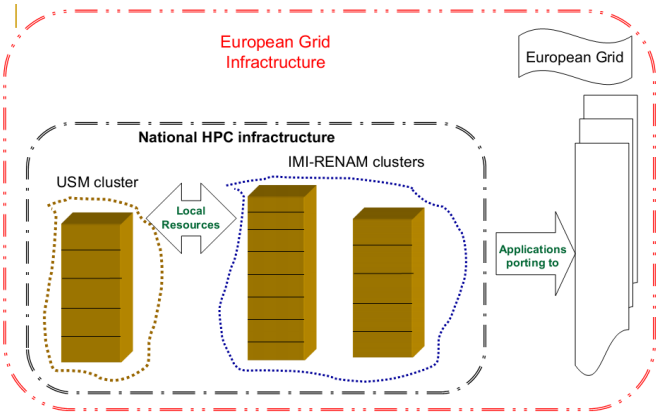

Figure 1. National Grid Infrastructure in Moldova.

The development of scientific clouds is a rather new, but perspective direction of computational technologies development. For Moldova the needs in cloud computing technologies deployment were analyzed during execution of SEERA-EI project ("South East European Research Area for eInfrastructures") funded by EC ERA-NET Programme. The carried out analysis had shown strong interest of the regional

and especially Moldovan research communities in scientific clouds technologies deployment.

For finding optimal solutions for scientific clouds deployment in the region of the South-East Europe were carried out investigations within SEERA-EI project. On the base of these work it was proposed to launch regional Pilot Call for projects in the area of scientific cloud computing. One of the Pilot Call priority topics was the feasibility study of approaches of scientific clouds infrastructures and technologies development in the region.

The study of available and developing in Europe clouds platforms for non-commercial use had shown that there are many offers developing due to the support of various international projects. We examined results of several project that had aim to elaborate technological solutions acceptable for open cloud infrastructure deployment. This allowed obtaining of some useful and interesting outcomes for practical utilization. The analysis of the following projects related to scientific cloud computing was produced:

- Enabling Clouds for e-Science (ECEE) Initiative, supported by NRENs and other partners in Europe. The project activities based on close collaboration on Grid computing, to extend it into cloud computing. ECEE has the aim to leverage national cloud infrastructures for Europe – there is a series of similar projects widening the initial EGEE initiative. The Initiative comprises VENUS-C project co-funded by European Commission, as one of six European Distributed Computing Infrastructures (DCIs). VENUS-C combines experiences in Grid infrastructures and Cloud computing to capitalize on EU investments. VENUS-C brings together 14 European partners and supports the following basic research disciplines: biomedicine - integrating widely used tools for bioinformatics, system biology and drug discovery into the VENUS-C infrastructure; data for Science - integrating computing resources through VENUS-C on data repositories.
- StratusLab – EC FP7 funded project that unites organizations from France, Greece, Switzerland, Spain and Ireland. The project enhances Grid infrastructure with virtualization and cloud technologies. The focus is on developing a complete, open-source cloud distribution that allows grid and non-grid resource centers to offer and to exploit an "Infrastructure as a Service" cloud concept.
- GRNET eScience cloud project further transformed to "~Okeanos" project that has the aim to offer virtualization and storage services for the Greek scientific community. The project strategy is gradual offering of services, starting with shared storage, moving to VM on demand, and then SaaS. The project policy background is existing MoU in place for Grid computing that now is expanding for HPC as well.
- OpenNebula.org initiative that is an open-source project aimed at building the industry standard and open source Cloud computing tools to manage the complexity and heterogeneity of distributed data centers infrastructures.

The main goal of the analysis of existing initiatives in the area of scientific clouds is the determination of optimal technological solutions for: finding standard platform to facilitate the interoperability; the integration of existing virtualization layers with the on-demand delivery model typical for commercial clouds; the virtualization and service-orientation supporting the better resource utilization, increased flexibility and enhanced provision of the user-focused environment; the governance models appropriate to driving open standards-based interoperability and integrated user services; funding models to support delivery of user-focused services leveling a cost-effective shared infrastructure provision.

The study performed allowed to formulate clear work programme for the elaboration of solutions and planning the deployment of interoperable Scientific Cloud infrastructure that consequently can be integrated to other cloud infrastructures like the Governmental M-Cloud initiative in Moldova.

III. Networking Support of the Computing Infrastructures Operation

To ensure effective operation of the national computing infrastructure the basic NREN infrastructure and its organizational structure has to be adjusted to support requirements and needs of the computational e-Infrastructure. These specific requirements refers to configuration of the national networking backbone operation and to its interrelations with external regional and more general European level networking segments that are providing the similar services and uniting common computational infrastructures.

Specific requirements of network operation are mainly focusing on [8]:

- creation of networking segments that offering the necessary level QoS;
- ensuring the necessary level of computational e-Infrastructure operation securing.

Distributed computing infrastructures as Grids and clouds are very critical to QoS parameters like guaranteed network bandwidth and optimized network latency. To achieve the necessary QoS parameters all national Grid sites integrated in the common VLAN and have prioritize access to the network.

There is no problem to make the necessary configuration in the internal NREN backbone. More complicated task is to make required configuration for regional or Trans-European Grid and cloud infrastructures. The most simple and convenient solution for implementation of similar approach at regional level can be using of cross border fiber connections that uniting neighbor NRENs and can be used for flexible networking segments configuration. Another approach to achieve the requested result is to use specific services implemented and proposed by GEANT network. However, this approach requires from all participating NRENs that are hosting common regional e-Infrastructures components to have the perfect connection to GEANT backbone and implement the respective set of networking services. Using GEANT services is more universal approach that has perspectives in future, but

now it requires additional investments and can be considered as more complicated and expensive solution.

Approaches for achieving the necessary level of computational infrastructures security dealt with permanent updating of the used middleware, system software of surrounded servers' and networking environment. This requires attracting qualified personnel for administration of clusters' and network equipment, elaboration and implementation of comprehensive rules that determine interrelations of NREN's NOC, local networks administrators, technical specialists and managers responsible for computational resources operation.

As important component for supporting of the joint networking – computational infrastructures securing is optimization of CERT functioning that initially was created for serving only as networking CERT. Creation of the same CERT structures are obligatory for European Grid and HPC infrastructures. To optimize secure incidents infrastructure operation and exclude duplication of efforts we decided to extend responsibility of the NREN CERT to monitor operation also of the existing computational infrastructures. This required integrating existing CERT to various security incidents monitoring structures and complying with their regulations.

IV. Education and Retraining of Users' Communities

Very important activity for effective use of computing infrastructure is permanent training of users' communities. For ensuring effectiveness of training activities within STCU project "Instrumental support for complex applications porting to the regional HPC infrastructure" was adapt and install instrumental open source software that is used for elaboration of interactive - training and users' education programs. We examined various open source packages that include Learning Management Systems (LMS) to support the elaboration of interactive training courses and on-line collaboration tools for organization interactive presentation and dissemination of material. As LMS for studying, deployment and testing the following software tools were selected:

- Moodle - Modular Object-Oriented Dynamic Learning Environment;
- Sakai;
- ILIAS (with Scorm editor).

As an interactive collaboration tool for educational web conferences organization was deployed the open source package BigBlueButton (BBB).

After preliminary studies and analysis it was decided to focus efforts on deployment of two popular LMS – Moodle and Sakai. The selected tools were installed on the local HPC systems at the Faculty of Mathematics and Informatics of the State University of Moldova and in the Institute of Mathematics and Computer Science of ASM. After experiments with this open source software we have begun the necessary procedures for transferring existing in the State University of Moldova training and teaching curricula to organize their interactive operation and on-line access. The accumulated experience allowed determining the ways of organization of the selected LMSs practical operation, future development and approaches for elaboration of new training programs that will be developing and operating interactively.

Moodle LMS package is suitable for the organization of traditional distance learning courses, as well as support for full-time study. Continuation working with Moodle has showed that for the correct delivering of training courses requires monitoring and intervention of the coach/teacher. It is important that LMS Moodle allows creating different types of accounts - entering the administrator and users with limited rights. Further works with Moodle were focused on creation of the integrated operational complex containing LMS Moodle and interactive collaboration tool BigBlueButton. The problem of integration of these packages was solved by combining them using virtual machine running Ubuntu 12.

The tests were organized and experiments produced for Big Blue Button web-conferencing package load threshold testing. Up to six subscribers were working properly. Experiments discovered that moderation of the conferences is mandatory. To improve the stability of the deployed version of BBB we prepared recommendation to replace the built-in package FreeSwitch on Asterisk that is having the similar functionality.

There were studied the structure and methods of use of LMS Sakai. Analysis of the Sakai functionalities shows that LMS can be applied for creation of interactive courses for HPC users' training. For real time (on-line) trainings organization that are using Sakai software it is convenient to integrate it with the web-conferencing system like BBB.

Proposed integrated software solutions based on open source packages were adapted to run on the existing computing resources of the two local multiprocessor clusters. Produced examinations and experiments allowed concluding that these instrumental toolkits are suitable for implementing various interactive training courses needed for potential parallel applications developers.

During experimental works with training content elaboration and delivering we determined the directions of the selected tools further adjustment and development:

- LMS Moodle suitable for the organization of traditional distance learning courses, as well as support for full-time study. However, to raise flexibility for this LMS is necessary creating different types of accounts - entering the administrators and users with limited rights.
- There was modified interface of interactive tool BigBlueButton in order to create closed web-conferences and add facility to record web-conferences.
- We worked on implementation of collaborative and knowledge systematization tools after receiving and analyzing various feedbacks from training users.

For preparing effective collaborative media and for elaboration of interactive - training programs we needed to solve the following issues:

- On line collaboration including notification of incidents, identifying and solving problems;
- Accumulation and systematization of knowledge on technological issues for of interactive training

organization and of the training projects execution in general;

- Creating and maintaining up to date database of interactive-training hardware and software (and more wider - hardware and software for applications execution);
- Creating a database of instructions and processes to support interactive-trainings projects creation, operation and support other works with users (Service HelpDesk)
- ServiceDesk as customers' support instrument - main objectives of the Service Help Desk are registration of decisions and tracking of incidents. The Service Desk has wider functions (e.g., requests for change, etc.) and can perform more extensive actions instead of just technical support of customers. It includes many other valuable features related to users' support, like issuance of digital certificates for work in Grid, etc.

After analyzing the existing commercial and Open Source software in the field of support of collaborative activities and systems to support relations with users (Atlassian Jira, Kayako, Spiceworks, ManageEngine, Mantis, Redmine with CRM and HelpDesk), it was decided to deploy the OTRS (Open-source Ticket Request System) with add-ons OTRS ITSM (IT Service Management).

All proposed software solutions are based on open source packages and we adapted them to the available computing resources. Produced examinations allow concluding that these instrumental toolkits are suitable for implementing various interactive training courses needed for all potential parallel applications developers.

V. Conclusions

Development of e-Infrastructures and associated technologies in Europe contributes to speeding-up of creation of high-performance and distributed scientific computing environments in Moldova. Now computing infrastructures are considering as a powerful tool for solving a wide range of complex problems of mathematical modeling and supporting of development of modern educational processes. The paper outlines the experience of development and use of computer infrastructures and services in Moldova and in the South-Eastern Europe region for solving complex simulation problems that require large amounts of computing resources.

Established computing environment can be adapted to solve wide range of scientific, educational and industrial problems that raising in various organizations and users' communities. It can serve as a fundamental basis for development of scalable complex applications that now have ability to be ported to capacitive computational resources of European and South-East Europe regional computational infrastructures.

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