IT-infrastructure as a basis of innovative development of science and industry

Andrii Malenko

Glushkov Institute of Cybernetics
of National Academy of Sciences
of Ukraine

Andrii Golovynskyi

Glushkov Institute of Cybernetics
of National Academy of Sciences
of Ukraine

Valentyna Cherepynets

Glushkov Institute of Cybernetics
of National Academy of Sciences
of Ukraine

1. INTRODUCTION

Today supercomputer technologies are considered as the most important factor for competitiveness of economy. Therefore, the advanced countries are developing new progressive ICT platforms for science – grid and cloud infrastructures with powerful supercomputer centers connected by an ultrafast communication channel.

At the present stage of scientific development, more attention is paid to the subtle effects and phenomena. Majority of prominent results, obtained at the forefront of science, are directly related to advances in computer technologies: Large Hadron Collider, nanotechnologies, genetics, chemistry, etc. The modern economy poses great challenges to manufacturers in energy efficiency, reliability and price of their products. One of the promising ways for innovative high-tech industries, including aviation, is the use of HPC and grid technologies.

In this paper we present achievements of IT-infrastructure for science in Ukraine: Ukrainian National Grid and Supercomputing Center of NAS of Ukraine.

2. UKRAINIAN NATIONAL GRID (UNG)

In Ukraine there are about 40 computer centers. Most of them are located at research institutions and universities. They provide research computing resources to various research organizations and educational institutions for training students of HPC specialties.

Computing centers of Ukraine are connected into Ukrainian National Grid (UNG) [1].UNG is a grid infrastructure, which shares the computer resources of the institutes of National Academy of Science and universities. Clusters function as a single network and have common authorization system – grid-certificates. For scientists it means a flexible choice of resources according to their research topic and software needs.

The principel task of the UNG is to develop the distributed computing and grid technologies to advance computational calculations of fundamental and applied science. Besides, UNG has to ensure a participation of the Ukrainian scientists in various major international Grid projects.

Ukrainian National Grid is supported by the targeted state scientific program financing development of grid-technologies, adopted by Ukrainian Government in 2009. The project goal is the creation of national grid-infrastructure and wide implementation of grid-technologies in all areas of scientific, social and economic activities in Ukraine, as well as training specialists on grid-technologies.

Currently grid infrastructure incorporates resources of 38 computing clusters of research institutes and universities with over 3100 total cores and available disk space 250 TB. The majority of clusters uses ARC and gLite middleware.

All grid sites are interconnected by a ring topological structure with multiple 10 Gb/s data channels. Academic network is also connected to the International Traffic Exchange Network through four 10 Gb/s data channels. For clusters taking part in CMS and ALICE experiment and having status of Tier-2 CERN the bandwidth up to 1GBit/s is guaranteed [2].

An important factor of rapid development and popularization of grid technologies in Ukraine is the presence of large computing resources in UNG. According to statistics, the usage of grid technologies in UNG shows steady growth since 2010.

The main efforts of recent period were aimed at harmonization of Ukraine's grid infrastructure to EGI requirements. In 2011 negotiations with EGI.eu project governing body started about integration of UNG into EGI. "Memorandum of Understanding" between EGI.eu and UNG was finally signed in November 2011. In July 2012 Ukrainian Grid Initiative of Ukraine (NGI_UA) completed the certification process for major grid services and became a full member of EGI team.

Due to the development of grid technologies and EGI membership Ukraine was able to participate in international projects in high energy physics (CERN), global climate change modeling, new medicine search, etc.

3. NATIONAL RESOURCE CENTER OF GLUSHKOV INSTITUTE OF CYBERNETICS

Glushkov Institute of Cybernetics (GIC) of National Academy of Sciences of Ukraine [3] is a world-recognized scientific center for solving fundamental and applied problems in computer science and engineering. GIC is the leading computer science research institute of National Academy of Sciences of Ukraine. It was founded in 1957 as a Computing Center of the Academy of Science of Ukraine on the base of the Lebedev's computer lab which had developed the first Soviet computer in 1950.

Founder and the first director of GIC academician Victor Glushkov (1923-1983) is worldwide recognized as a pioneer of the computer era (IEEE Computer Pioneer Award for digital automation of computer architecture).

GIC has vast experience in the development of technological components of information society policy in Ukraine. Besides, GIC is involved in the preparation of materials for a high level international collaboration in the information society area.

One of the most important recent achievements of GIC is the development and construction of supercomputer family "SCIT" (Supercomputer for Intellectual Technologies) [4]. SCIT family includes four computing clusters.

The hybrid supercomputer "SCIT-4" developed in 2012 is currently the top performance and the most "green" HPC system in Ukraine [5].

To fulfill the increasing needs of Ukrainian scientists the National Resource Center for UNG was created in Glushkov Institute of Cybernetics on the basis of supercomputer SCIT. Today the resource center SCIT with 1000+ CPU cores, NVidia Tesla accelerators and 100 TB grid storage provide the largest amount of UNG computational and storage resources. Total usage of SCIT supercomputer in 2012 was 5 million processor hours. In 2012 grid users submitted more than 45000 jobs. The reliability of SCIT services for grid computing was 99.8%. Overall reliability index for SCIT computing services reached 99.93%.

National Resource Center provides computing resources and grid services to all virtual organizations of UNG. Main virtual organizations of UNG:

- CompuChemGridUA – quantum chemistry
- GEOPARD – calculation of three-dimensional full-wave seismic models in grid environment, studies of radiation-stimulated processes, phase transformations and isomorphic substitutions in mineral structures related to the tasks of nano-mineralogy and radiation
- MatModEn – mathematical modeling in energy
- Medgrid – medical grid system for population studies in cardiology
- MolDynGrid – molecular biology
- Multiscale – wide range of scientific and applied problems that require a multi-faceted approach, from the quantum-chemical calculations and ending mesoscopic level modeling
- SysBio – upgrade of gene regulation networks
- VIRGO.UA – cosmology and astrophysics.

4. INTERNATIONAL COLLABORATION

The availability of powerful resources and advanced infrastructure allows Ukraine to actively participate in international projects. Ukrainian specialists act as active developers of supercomputer technologies, collaborating with various institutes and companies from outside Ukraine in the following areas: middleware for ARC (Sweden, Norway), gLite (CERN), schedulers (RSC, Russia), intellectual monitoring and control, cloud platforms, new programming paradigms, advanced computational methods for hybrid computing platforms.

Among the results of such collaboration we should mention the SCMS project [6], an open source platform for e-science. It combines versatile cluster management, user administration with general purpose GUI for running parallel tasks in distributed computer environments. Project was intended to bring computational quantum chemistry, molecular dynamics, fluid dynamics, etc. to the next level.

Development of grid in Ukraine resulted in appearance of domain specific international research communities on the basis of virtual organizations of UNG. MolDynGrid virtual laboratory [7] is one of the most successful international collaboration for interdisciplinary research in computational structural biology and bioinformatics. The goal of this VO is to develop an effective infrastructure for conducting in silico calculations of molecular dynamics of biological macromolecules in water-ion environment in 100 ns timescale.

For emerging industries to solve the applied problems virtual laboratories are created on the basis of supercomputer centers. A virtual laboratory of hydro- and gas dynamics modeling was created at Supercomputer Center SCIT as a joint effort of Ukrainian-Russian collaboration [8]. The use of modern supercomputers and special software significantly reduces the number and duration of field testing at all stages of development, research, aero-and hydrodynamic properties of the product, test construction for durability and reduced energy creation stands specimens and physical models.

Use of grid and cloud technologies made possible processing and storage of extra large volumes of medical data within VO Medgrid, devoted to the storage medical analysis data and population research in cardiology [9].

5. CONCLUSIONS

IT infrastructures are one of the priority directions of development of Ukrainian science. They are actively harnessed in various scientific research areas and make possible fruitful international collaboration. Ukrainian specialists are widely involved in development of IT research platforms which are used to solve contemporary problems.

Ukrainian HPC community annually holds an international conference in informatics and is actively involved in various academic forums around the world.

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