eInfrastructure in the Czech Republic

Luděk Matyska

The Czech national eInfrastructure, as defined in the Roadmap of the Large Scale Research Infrastructures for Czech Republic, is being built and operated by three major players -- CESNET (Prague) and centers CERIT-SC (Brno) and IT4Innovations (Ostrava) -- and encompasses all the services from physical and logical network, grid and cloud computing, data storage and high performance computing systems. With the network and grids already in operations, clouds and large scale data storage under deployment, CESNET and CERIT-SC are closely collaborating to provide a unique and highly flexible distributed environment. Its principal technical features as well as some operational results will be presented in the lecture.

Activities and visions in the Italian grid infrastructure

Mirco Mazzucato

The Italian national grid: IGI
The relations with the European Grid Initiave – EGI
The European Middleware: gLite and EMI
Possible future directions for the Distributed Computing Infrastructures in Europe

The Italian Grid Initiave - IGI develops, maintains and operates, on behalf of the constituent organizations and with the aims to satisfy the need of the reference research user communities, the services of the national grid infrastructure which enable, through agreed policies at regional or international level, the remote acquisition, access and sharing of the ICT resources made available by the IGI shareholders or IGI itself.

At the end of 2010 IGI, currently a Joint Research Unit lead by INFN, has received by the Italian Ministry of University and Research- MIUR a “sustainable line of budget” to constitute a new legal organization pursuing on a more solid base the above objectives.

This talk gives an overview of the model and the organizational structure IGI is now developing for providing and consolidating the offer of the grid services required by the research communities. The strategy adopted by IGI to smoothly integrate a Cloud offer without any change in the current center popular best practices, based on the successful batch systems for the machines management, will be presented together with the expectations for an efficient integration with the EGI offer.

IGI is deeply involved in EMI. The status and future of some key components will be discussed together with the IGI vision for the future sustainability of the European Open Grid and Cloud Middleware software and of EGI itself.

GPGPU Applications in Theoretical Chemistry

Stanislav Biskupič

General purpose computing on graphical processing units, known as GPGPU (or now often referred to as GPU computing), is the approach of performing computation on the GPU instead of the CPU. GPU computing has been made possible by the increasing programmability and performance of GPUs.

The accuracy and extensibility of computational chemistry methods, particularly those which approximately solve the Schrödinger equation, are ultimately limited by the speed at which computer processors can execute floating point and memory operations. Due to fundamental limitations in processor technology, clock speeds are not significantly increasing, and all future increases in computational capability are expected to come from parallelism, which now more than ever can be found within a single processor. Graphics processing units (GPUs) are a type of massively parallel processor in which hundreds of cores can execute many instructions at once, provided they are sufficiently regular. Recently, many theoretical chemistry groups have demonstrated the incredible power of GPUs for scientific applications when sufficient effort is devoted to programming them to exploit their high degree of instruction-level parallelism. The programmability of GPUs has increased dramatically with the NVIDIA CUDA API and associated SDK including CUBLAS and CUFFT (together with other GPU oriented linear algebra libraries e. g. CULA or MAGMA), although these tools require more programming effort to realize the same relative performance as CPUs, especially for irregular algorithms.

To date, many quantum chemistry methods have been implemented on GPUs, including classical molecular dynamics, 2-electron atomic integrals, DFT and SCF, perturbation theory, and quantum Monte Carlo.

An overview of the Finnish model for provisioning of services for scientific computing and its extending to pan-European e-infrastructures

Per Öster

CSC - IT Center for Science Ltd, a Finnish information technology centre for research, provides modelling, computing and information services for academia, research institutes, the public sector and industry. CSC has also wide activities in data management and maintains Funet, the Finnish university and research network that also connects Finland to NORDUnet and GEANT. CSC is a limited non-profit company. The shares are fully owned by the Finnish state, and governed by the Finnish Ministry of Education and Culture. CSC is the largest national computing centre in Northern Europe with a staff exceeding 200. This talk gives an overview of the Finnish model for provisioning of services for scientific computing and how the national program extends to the pan-European e-infrastructures of EGI, PRACE, EUDAT and other research infrastructures (ESFRI).

Final program:

Monday	24.10.2011	13:00 – 13:30	Registration
		13:30 – 14:00	Opening session
		14:00 – 14:45	**Invited lecture** ***Luděk Matyska***
		14:45 – 15:30	**Invited lecture** ***Mirco Mazzucato***
		15:30 – 16:00	Coffee break
		16:00 – 16:45	**Invited lecture** ***Stanislav Biskupič***
		16:45 – 17:30	**Invited lecture** ***Per Öster***
		17:30 – 18:30	**Panel discussion**
		18:30	**Reception**
Tuesday	25.10.2011	9:00 – 9:40	Invited lecture
		9:40 – 10:20	Session 1
		10:20 – 10:35	Coffee break
		10:35 – 12:15	Session 2
		12:15 – 13:00	Lunch
		13:00 – 13:40	Invited lecture
		13:40 – 15:20	Session 3
		15:20 – 15:35	Coffee break
		15:35 – 17:15	Session 4
		17:15 – 18:15	Session 5
Wednesday	26.10.2011	9:00 – 10:20	Special session Crisis 1
		10:20 – 10:35	Coffee break
		10:35 – 11:55	Special session Crisis 2
		11:55 – 12:40	Lunch
		12:40 – 13:40	Tutorial on Cloud computing
		13:40 – 13:55	Coffee break
		13:55 – 15:15	Special session Recler 1
		15:15 – 16:15	Special session Recler 2
		16:15 – 16:30	Consortium "SlovakGrid"
		16:30 – 17:00	Program committee meeting
		17:00	Closing ceremony

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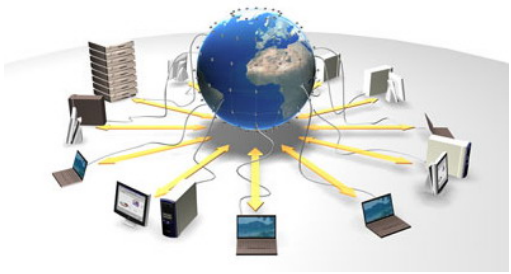
7th International Workshop on Grid Computing for Complex Problems GCCP 2011

October 24-26, 2011
Institute of Informatics, Slovak Academy of Sciences, Bratislava, Slovakia
Website: http://conference.ui.sav.sk/gccp2011/



The yearly meeting place of top researchers and practitioners in e-Science related to Grid Technologies, GCCP is one of the largest conferences in Central Europe in its area organized on a yearly basis, where many top researchers are regularly presenting their work. During its previous 6 years of existence, 30 distinguished keynote speakers were invited to attend and share their knowledge, thus reinforcing GCCP quality.

The aim of the conference is to inform the wide professional public, special and scientific workers from industry, research institutions, Academy of Sciences, project and supplying organizations, and technical universities and high schools about the newest knowledge in the area of grid computing and to ensure exchange of their experience.

We invite researchers and scientists interested in distributed high-performance computing to attend **invited lectures** given on **Monday, October 24, 2011** at **14^{00}** in the great hall of the SAS. After the presentations, a **panel discussion** will be organized, which may continue during a **reception**.
Attendance to the first day events of the workshop is **free of charge** (for organizational reasons, please register by e-mail conference.ui@sav.sk up to October 17, 2011).