



Contribution ID: 88

Type: **Poster contribution**

## Application Identification and Support in BalticGRID

*Wednesday 1 March 2006 18:30 (20 minutes)*

### Introduction

The Baltic Grid project, a FP6 program, involving 10 leading institutions in six countries, started in November 2005. Its aims to i) develop and integrate the research and education computing and communication infrastructure in the Baltic States into the emerging European Grid infrastructure, ii) bring the knowledge in Grid technologies and use of Grids in the Baltic States to a level comparable to that in EU members states, and iii) further engage the Baltic States in policy and standards setting activities. The integration of Baltic States into the European Grid infrastructure is primarily focusing on extending the EGEE (with which four partners are already engaged) to the Baltic States. The Baltic Grid takes advantage of the local existing e-infrastructures in the region.

The Baltic Grid project is of high strategic importance for the Baltic States and it is designed to give a rapid build-up of a Grid infrastructure, contributing to the enabling of the new member states participation in the European Research Area. One of the most important steps in Baltic Grid development is application identification and support. This activity will be carried out through three tasks.

### Pilot Applications

Baltic Grid intends to initiate three pilot applications for validation and for demonstration of successful scientific use.

High-energy physics application includes statistical data analysis, production of Monte Carlo samples and distributed data analysis, nuclear and sub-nuclear physics, condensed matter physics and many-body problems. It will be implemented because of the critical importance of Grids to this community and its relative maturity.

Material sciences application presents research areas, having substantial number of potential Grid users among scientists in Baltic states. It includes tools for establishing the geometrical structure of various organic, metal-organic and inorganic materials; understanding optical and magnetic properties of molecular derivatives; predicting new technology and creation of new materials with specified characteristics. Modelling and simulation of heterogeneous processes in chemistry, biochemistry, geochemistry, electrochemistry, biology, engineering will be implemented because of MS strategic importance to the Baltic States and substantial computing needs.

A bioinformatics application will be implemented to give tools and computing procedures for sequence pattern discovery and the gene regulatory network reconstruction, inference of haplotype structure and pharmacogenetics related association, studies, modelling and exploration of mechanism of enzymatic catalysis, de novo design of proteins, quantum-mechanical investigations of organic molecules and their applications, for the refinement of 3D biological macromolecule models against X-ray diffraction or NMR data, for modeling of biosensors and other reaction-diffusion processes. This application intends also to support the collaborative

efforts of scientists in the Baltic States in this highly distributed community with needs to share data from many sources and a diverse set of tools.

#### Special Interest Groups

The task of special interest groups (SIG) aims to improve communication among many separate research groups, having similar or related R&D interests. The development and implementation of SIGs is a relatively new idea in grid computing infrastructure based on semantics representation methods and tools and leading to enhancement of services and applications with knowledge and semantics. Research areas under consideration for SIG development and implementation are: modelling of the Baltic Sea eco-system (together with BOOS –a future operational oceanographic service to the marine industry in the Baltic region), hydrodynamic environmental models for sustainable development of the Baltic Sea coastal zone, environmental impact assessment and environmental processes modeling, life sciences and medicine.

#### Application Adaptation Support

This is a specific activity aiming to organize and initiate communication between application experts and Grid experts facilitating rapid Grid adaptation and deployment of applications through formation of an Application Expert Group. This group will analyze applications and identify required Grid technologies and provide consulting services to application developers. The services will include assistance with integration with the Migrating Desktop to enable GUI-based access to the BG infrastructure and services, ensuring interoperability with the BG middleware. Performance studies to find bottle necks of the deployed applications may be carried out if needed using tools for performance evaluation, like G-PM and OCM-G, developed in CrossGrid Project.

**Author:** Dr JUOZAPAVICIUS, Algimantas (associate professor)

**Presenter:** Dr JUOZAPAVICIUS, Algimantas (associate professor)

**Session Classification:** Poster and Demo session + cocktail

**Track Classification:** Poster session