Applications in BalticGrid

www.balticgrid.org
sig.balticgrid.org

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- **BalticGrid (BG) project extends the European Grid by integrating new partners from the Baltic States (Lithuania, Latvia and Estonia) in the European Grid research community.**

- **BG fosters the development of Grid infrastructure in these countries.**

- *BalticGrid project started on 1 November 2005 and is a 30-month effort.*

- **Enables scientists in the Baltic States to participate efficiently in the European Research Area.**

- **Develop and establish Special Interest Groups (SIGs) in significant application areas.**

- **Promote the Open Source Community by making of Open Source Software for the BalticGrid.**

- **KTH (Sweden)**

- **EENET (Estonia)**

- **Research institute NICPB (Estonia)**

- **IMCS University of Latvia (Latvia)**

- **Riga Technical University (Latvia)**

- **Vilnius University (Lithuania)**

- **Research institute ITPA (Lithuania)**

- **Research institute IFJPAN (Poland)**

- **Poznan Super computing national center (Poland)**

- **CERN (Switzerland)**

Cross-project communities

- Lithuanian researches cooperation in ITER (International thermonuclear fusion experimental reactor).

Selection criteria

New application meets light peer review evaluating:

- Scientific impact
- User community
- Infrastructure

Research areas in BalticGrid

- **Pilot applications**
  - **High energy physics**
  - **Material sciences**
  - **Bioinformatics**
- **Special Interest Groups (SIGs)**
  - **Baltic Sea Eco-System Modelling**
  - **Text Annotation Service**
  - **Text-to-Speech Service**
  - **Stellar Spectra Computation**
  - **Atomic and Nuclear Computations**
  - **Computational Modelling of heterogeneous Processes**
  - **Multidimensional scaling**
  - **GAMESS (modeling of chemical, physical and biological processes)**

- Application support
  - Application expert group
  - Migrating desktop, gridcom
  - Performance evaluation tools (G-PM, OCM-G)

High Energy Physics (HEP)

- *Compact Muon Solenoid (CMS)* - is designed as a general-purpose detector, studying many aspects of proton collisions, contains subsystems which measure the energy and momentum of photons, electrons, muons, and other products of the collisions.

- *Large Hadron Collider Beauty (LHCb)* - helps to simulate particle events in Large Hadron Collider, produces Monte Carlo data in the same form as a real collider detector.

NEW:

- Applications are implemented by supporting the existing VOs (in EGEE);

- Attracted HEP research groups in Baltic States, very intensive usage of grid resources;

- Statistical data analysis, based on HEP methods, is now applied to other areas of modeling.

Material Science

- *GAMESS and Dalton* (also MolPro and others, in addition) - large scale modelling of the kinetics of meta-stable systems with application to advanced electronic materials, condensed matter physics, computes the energy of an assembly of nuclei and electrons placed in a repeated cells.

- Applications are now separated into VO – GAMESS, attracted numerous users as soon as they were implemented.

- New: The scope of research is now much broader:

  - computing of nano-scaled objects (separate research project emerged - GridTechno).

  - Vilnius Parallel Shell Model Code (VPSM), also will be implemented as SIG.

  - GAUSSIAN software is now used (in addition);

Bioinformatics

- **Applications for modeling biosensors and other reaction-diffusion processes;**

- **Applications for DNA sequence pattern discovery and the gene regulatory network reconstruction (Bash shell, Perl, archiving tools, storage of data)**

- **Set of common purpose Bioinformatics applications (can be used as subroutines or utilities)**

- **NEW: having large computing resources is really worth and essential to expand the scope of research**

Special Interest Groups

- *Text annotation* (syntactic parser for Latvian, applied to the text corpus to get linguistic annotation) - **expands to other languages;**

- *Text-to-speech* (solving prosody modeling problem for Lithuanian language) - **expands to other linguistic studies;**

- *Baltic Sea Eco-system modeling* (analysis for ecological-hydrodynamic model based on finite elements) - **expands to sea operational models;**

- *Computer modeling* (application for computer simulation of electric field in phospholipidic membranes, the originating problem seeks understanding of Alzheimer's and Parkinson's diseases; based on various solvers for numerical algebra and differential equations, application to biochemistry, electrochemistry, etc.) - **expands the scope of research.**

Special Interest Groups

- *Nuclear and atomic* (analysis of spectral characteristics of highly charged ions, Nuclear shell model with core) - the research expands and turns out to some ITER research topics;

- *Stellar spectra* (modeling of stellar atmosphere) - expanding to large projects, like models of chemical evolution of galaxies.

SIGs expand in topics, in the scope of research, and in number of users.

Gridification guides

■   Detailed Tutorials on development of grid applications are available:

http://sig.balticgrid.org/tutorials/

■   Users having any problems, questions or need information generate a ticket (*support@balticgrid.org*).

The ticket is not closed until user confirms he is satisfied.

Conclusion on applications

- **More than 20 scientific publications.**

- **Applications grouped by topics, similarity and used methods.**

- **Special Interest Groups formed and new are planed.**

- **High Energy Physics applications CMS and LHCb selected, they also include libraries and possibilities for statistical data analysis (especially analysis based on Monte Carlo).**

- **Material sciences: VO GAMESS established (for licensing rules to be solved), DALTON selected, other applications determined.**