



BalticGrid Project



NA3: Application Identification and Support

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Objectives:

- identify application groups and communities that can benefit from the BG infrastructure and services,
- identify the needs of those groups and communities,
- establish Special Interest Groups for those groups and communities,
- develop proficient and successful user communities by working with other BG activities to address the needs of the application groups





Tasks:

■ Task 1: Pilot applications

- ▶ high energy physics
- ▶ material sciences
- ▶ bioinformatics

■ Task 2: Special Interest Group

- ▶ Baltic Sea Eco-System Modelling
- ▶ Text Annotation Service
- ▶ Text-to-Speech Service
- ▶ Stellar Spectra Computation
- ▶ Atomic and Nuclear Computations
- ▶ Computational Modelling of heterogeneous Processes

■ Task 3: Application support

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





Task 1:

■ **High Energy Physics**

- **CMS – to generate Monte Carlo datasets, simulation and reconstruction (implemented by joining the corresponding VO of EGEE)**
- **LHCb - simulation software for LHCb experiment, producing Monte Carlo data in detector's form (implemented by joining the corresponding VO of EGEE, testing the BG)**
- **statistical data analysis and production of Monte Carlo samples, distributed data analysis**





Task 1:

■ Material Science

- GAMESS – a well established set of applications, is now managed by a separate VO – Gamess, also has a potential to attract numerous users
- in the process of implementation
 - ▶ NSBGT (*multicomponent geochemical transport models*)
 - ▶ ABINIT (*condensed matter physics, computes the energy of an assembly of nuclei and electrons placed in a repeated cell*)





Task 1:

■ Bioinformatics

- sequence pattern discovery and the gene regulatory network reconstruction,
- inference of haplotype structure and pharmacogenetics related association
- 3D biological macromolecule models against Xray diffraction or NMR data
- visualization of large sets of multidimensional bio data by means of multidimensional scaling





Task 2:

Special Interest Group (SIG):

- concept, being developed as an application in BalticGrid project (www.balticgrid.org)
- SIG is going to be implemented as a public service based on grid technology
- the main task of SIG is to enable group-to-group communication of scientists and researchers, having similar or related R&D interests (to create virtual spaces)
- the functionality of SIG is based on grid computing infrastructure, introducing new possibilities and features to a virtual space





Task 2:

Services for collaboration of SIG members:

- **Services accessible via internet browser (site created using Plone CMS):**
 - On-line forum
 - Mail-lists
 - On-line documents and data repositories
 - BalticGrid surveys, news, events etc.
- **Collaboration via Access Grid:**
 - Audio and video conferencing
 - Data and applications sharing
 - Computing sharing on-line





Task 2:

Navigation

Home

General Info

Special Interest
Areas

Services

Message Board

Main

Text-to-Speech

Text Annotation

Baltic Sea Eco-
System
Modelling

Stellar Spectra

Atomic and
Nuclear

Message Board

SIGBalticGrid Message Board

SIGBalticGrid

Forum name ▲

Main

Main Forum

Text-to-Speech

Text-to-Speech Forum

Text Annotation

Text Annotation Forum

Baltic Sea Eco-System Modelling

Baltic Sea Eco-System Modelling Forum

Stellar Spectra

Stellar Spectra Forum



Task 2:

Data repository in SIG

Advantages of using Plone Content Management System as data repository:

Easy access to data by using web browser. No additional installations are required to access data.

Access for data viewing could be given even for unregistered users, so more people could participate in SIGBalticGrid activities.

Disadvantages of using Plone Content Management System as data repository:

Data can only be viewed but can not be used on-line in collaboration with other members of SIGBalticGrid.

To line up: Plone Content Management System as data repository in SIGBalticGrid can be used for sharing any type of data that does not require on-line applications that use this data. That data could be: first of all publications, reports or any other special data.





Task 2:

Data repository in SIG

Advantages of using Access Grid as data repository:

Shared data can be not only viewed but also used by shared Access Grid applications, in other words data not only can be viewed but also modified and used collaboratively.

Disadvantages of using Access Grid as data repository:

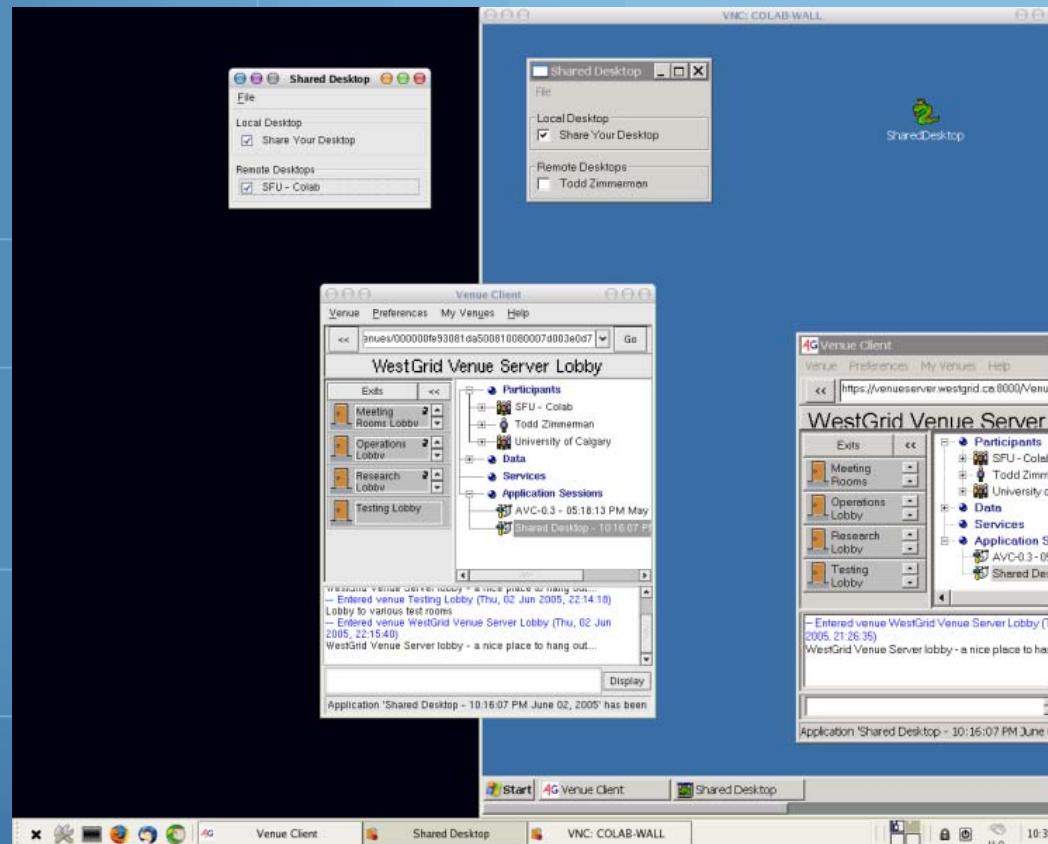
Access Grid Toolkit downloading and installation can make data sharing more difficult (i.e. when data is shared from different computers).

To line up: Access Grid as data repository in BG SIG can be used for sharing any type of data but primary for data that require on-line applications/computations that use this data.



Task 2:

- **Special Interest Groups (videoconferencing, screenshot sharing, shared desktop, shared pdf, etc.):**

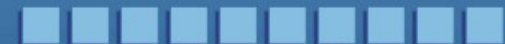




Task 3:

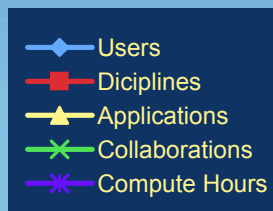
■ **Application support**

- **Application expert groups are for:**
 - ▶ **identification of grid techniques that should be used**
 - ▶ **grid-enabling procedures**
 - ▶ **deployment procedures**
 - ▶ **possibility of integration with user-friendly interface (Migrating Desktop)**
 - ▶ **possibility of using performance tools**
- **Migrating desktop – a common point for the project tools, resources and services**
- **Performance evaluation tools (G-PM, OCM-G)**





Targets



Target	Project month 12	Project Month 24	Project Month 30
Number of Users	7 40	100	150
Number of Disciplines	6 3	10	15
Number of Application Codes	5 3	6	20
Number of International Collaborations	4 10	20	40
Number of Compute hours per Year	3 1 x 10 ⁶	2 2 x 10 ⁶	4 x 10 ⁶