

APPLICATION AREAS FOR SIG ANALYSED

Document Filename: **BG-DNA3.6-ApplicationAreasForSIGAnalysed.doc**

Activity: **NA3**

Partner(s): **VU, IFJ PAN, EENet, NICPB, IMCS UL, PSNC, ITPA**

Lead Partner: **VU**

Document classification: **PUBLIC**

Abstract: The BalticGrid's deliverable DNA3.6 presents analysis of SIG application areas. The main task of SIGs is to enable the communication within a group of scientists and researchers, having similar or related R&D interests. SIGs are capable also to serve communication of group-to-group of scientists or just grid users (by creating virtual spaces). For such purposes special grid-based services for research groups and for the networking suitable applications were designed and organized into separate components. There were 6 different SIGs selected, satisfying the conceptual and technical requirements for users of BalticGrid.





Document review and moderation

	Name	Partner	Date	Signature
Released for moderation to				
Approved for delivery by				



Document Log

Version	Date	Summary of changes	Author
0.1	13/02/2007	Draft version	Linas Bukauskas
0.2	15/04/2007	Text added, content's revision	Margarita Kazakeviciute, Algimantas Juozapavicius
0.3	27/04/2007	Text updated, English improved	Algimantas Juozapavicius, Daiva Kaukeniene
0.4	30/04/2007	Final version, prepared for reviewing	Algimantas Juozapavicius

CONTENTS

1. INTRODUCTION.....	5
1.1. PURPOSE OF THE DOCUMENT	5
1.2. ABBREVIATIONS	5
2. EXECUTIVE SUMMARY	6
3. DESCRIPTION OF APPLICATIONS AREAS FOR SIG	8
3.1. BALTIC SEA ECO-SYSTEM MODELLING	9
3.2. TEXT-TO-SPEECH SERVICE	12
3.3. TEXT ANNOTATION SERVICE.....	12
3.4. STELLAR SPECTRA SERVICE	15
3.5. ATOMIC AND NUCLEAR COMPUTATIONS	18
3.6. COMPUTATIONAL MODELLING OF HETEROGENEOUS PROCESSES	20
4. CONCLUSSIONS	23

1. INTRODUCTION

The Baltic Grid project aims i) to develop and integrate the research and education computing and communication infrastructure of the Baltic States into emerging European Grid infrastructure, ii) to bring the knowledge in Grid technologies and use of Grids in the Baltic States to a level comparable to that in EU member states with a longer experience in the development, deployment and operation of Grids, and iii) to further engage the Baltic States in policy and standards setting activities. The integration of The Baltic States into the European Grid infrastructure will primarily focus on extending the EGEE to the Baltic States (with which four partners are already engaged).

The SIGs, suggested in BalticGrid project, have the main task to offer for users an intuitively well-defined interface, making the capability to run and manage jobs in the grid computing environment much easier. SIG aims to enable communication within a group of scientists and researchers, having similar or related R&D interests. SIGs are capable also to serve communication of group-to-group of scientists or just grid users (by creating virtual spaces). For such purposes special grid-based services for research groups and for the networking suitable applications were designed and organized into separate components.

1.1. PURPOSE OF THE DOCUMENT

The purpose of this document is to present the results of conceptual and technical analysis of SIGs, possible to be implemented in the BalticGrid project.

1.2. ABBREVIATIONS

BG – BalticGrid

HEP – High Energy Physics

MS – Material Science

SIG – Special Interest Group

2. EXECUTIVE SUMMARY

The main task of SIGs is to enable the communication within a group of scientists and researchers, having similar or related R&D interests. SIGs are capable also to serve communication of group-to-group of scientists or just grid users (by creating virtual spaces). For such purposes special grid-based services for research groups and for the networking suitable applications were designed and organized into separate components.

SIGs are being implemented as a public services based on grid technology:

- Services accessible via Internet browser (***sig.balticgrid.org***):
 - On-line forum ;
 - Mailing-lists ;
 - On-line documents and data repositories ;
 - Web based tool GridCom (the user can run and monitor grid applications through a web browser);
 - On-line BalticGrid surveys, news, events information, etc.
- Collaboration via Access Grid:
 - Audio and video conferencing (AccessGrid on accessgrid.sig.balticgrid.org or accessgrid.balticgrid.org or accessgrid.mif.vu.lt);
 - Data, file and applications sharing;
 - Computing sharing on-line.

Requirements for group of researchers to be defined as a separate SIG application area:

- The special interest group correspond to some research project or to some topic, and the users within group share application programs;
- The number of users within a group implies 3 researchers or more (usually 6 users);
- The number of users in SIG has a strong potential to increase;
- The topic of SIG represents an important scientific issue or is valuable to regional scientists;
- The SIG represents a service only possible to be implemented within grid technology.

This deliverable lists application areas for SIGs, that have been suggested by potential Baltic Grid users. The applications have been analysed for contextual correspondence with the pre-defined topics of application identification and classified in terms of corresponding subject and technical aspects. Such analysis is based also on generalized technical aspects, referring to computing environment.

According to the reviewing of suggestions of scientists in the Baltic States and the technical analysis of applications the following application areas for SIGs were chosen:

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

3. DESCRIPTION OF APPLICATIONS AREAS FOR SIG

The main task of SIGs is to enable the communication within a group of scientists and researchers, having similar or related R&D interests. SIGs are capable also to serve communication of group-to-group of scientists or just grid users (by creating virtual spaces). For such purposes special grid-based services for research groups and for the networking suitable applications were designed and organized into separate components.

SIGs are implemented as a public service based on grid technology. The functionality of SIG is based on grid computing infrastructure, introducing new possibilities and features to a virtual space.

The services for collaboration of BalticGrid members are provided as:

- Services accessible via Internet browser (the site *sig.balticgrid.org* is designed and implemented by using the content management system CMS, namely Plone):
 - On-line forum ;
 - Mailing-lists ;
 - On-line documents and data repositories ;
 - Web based tool GridCom (the user can run and monitor grid applications through a web browser);
 - On-line BalticGrid surveys, news, events information, etc.
- Collaboration via Access Grid:
 - Audio and video conferencing (AccessGrid on accessgrid.sig.balticgrid.org or accessgrid.balticgrid.org or accessgrid.mif.vu.lt);
 - Data, file and applications sharing;
 - Computing sharing on-line.

Requirements for SIG application. The users willing to form a special interest group or to be included into some SIG, have to satisfy following requirements:

- The special interest group correspond to some research project or to some topic, and the users within group share application programs;
- The number of users within a group implies 3 researchers or more (usually 6 users);
- The number of users in SIG has a strong potential to increase;
- The topic of SIG represents an important scientific issue or is valuable to regional scientists;
- The SIG represents a service only possible to be implemented within grid technology.

This deliverable lists application areas for SIGs, that have been suggested by potential Baltic Grid users. The applications have been analysed for contextual correspondence with the pre-

defined topics of application identification and classified in terms of corresponding subject and technical aspects. Such analysis gives a possibility to cluster applications into suitable topics, to compare applications, to cluster them into groups, and to make suggestions for their development and deployment in the Grid environment.

The applications have been analysed (the first analysis was done in the deliverable DNA3.1 – Application Support Road Map) and grouped according the following generalized technical aspects:

- type of source code, programming technology/languages, libraries;
- license agreement,
- minimal/maximal requirements for computer resources, including type of CPU, number of CPU in a node, number of nodes in a cluster; amount of RAM, aggregate and per node; bandwidth requirement on interconnect; minimal/maximal/ and recommended execution time for an application.

According to the reviewing of suggestions of scientists in the Baltic States and the technical analysis of applications the following application areas for SIGs were chosen:

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

3.1. BALTIC SEA ECO-SYSTEM MODELLING

The field of interest of this SIG is defined by hydrodynamic environmental models. These models present very useful tools to solve numerous environmental problems such as eutrophication control, sediment transport and coastal erosion control, salinity predictions, the fate of various harmful pollutants (for example oil), dredging and other harbours activities impact prediction etc. The majority of these problems are typical for Baltic countries. Development and application of these models requires considerable computing resources, therefore grid infrastructure is good promotional measure to organisations that are already working with these models. It also increases the number of users.

The potential users for this SIG are distributed, they are from the Vilnius University, Faculty of Natural Sciences; Research Institute of Physics, Vilnius; Klaipeda University; University of Latvia, Estonian Marine Institute.

Applications under analysis and considerations for technical specifications are:

- **SHYFEM:** Finite element hydrodynamic-ecological model. It is used for modelling physical (water currents, temperature, salinity) and ecological (eutrophication) processes in shallow water (lagoons and coastal areas):
 - Salinity Evaluation of the Baltic Sea Applying the Simple and Ordinary Lognormal Kriging
 - Spatial and Temporal Variation of Water Salinity in the Curonian Lagoon
 - Nitrogen Budget and Limitation in the Shallow Eutrophic Curonian Lagoon
 - Co-Variation Analysis of Water Quality Monitoring Data from the Curonian Lagoon
- **SWAN:** Simulating WAVes Nearshore software can be applied to nearshore wave modeling for harbor and offshore installation design, coastal development and management, wave hind casting.

General description of the application:

Scientific domain the application belongs to	<i>SWAN is a numerical wave model for obtaining realistic estimates of wave parameters in coastal areas, lakes and estuaries from given wind-, bottom-, and current conditions.</i>
Name of application	<i>Simulating WAVes Nearshore</i>
Short name of application	<i>SWAN</i>
Web site of application	<i>www.fluidmechanics.tudelft.nl/swan</i>
Goals of application	<i>Nearshore wave modelling for harbour and offshore installation design; Coastal development and management; Wave hindcasting.</i>
Architecture of application	<i>Single computer program</i>

The applications presented above may be used to solve environmental issues, as presented below.

- **Monitoring and Analysis:**
 - Monitoring of Marine Environmental Genotoxicity.
 - Environmental Monitoring of Water Quality in Coastal Sea Area Using Remote Sensing and Modeling.
 - Sea Ice Monitoring and Modelling in Small Bay.

- Space-Time Modeling of Baltic Sea Coastal Zone Characteristics.
- Discriminant Analysis of Spatial-Temporal Data Collected in the Lithuanian Economic Zone in the Baltic Sea.
- **Environmental and Ecological Issues:**
 - Impact of Soil Dumping on Lithuanian Fisheries in the Baltic Sea.
 - Use of Ferrybox Measurements for the Baltic Sea Environment Assessment.
 - Copepod *Limnocalanus macrurus* mating in relation to vertical migrations and aspects of feeding rates in the Bothnian Sea.
 - Studies of Environmental Genotoxicity in Offshore Zones of the Baltic and North Seas.
 - Cytogenic Damage in Perch (*Perca fluviatilis* L.) Exposed to Crude Oil.
- **Information Systems:**
 - Information System for Data from Marine and Transitional Waters.
 - BOOS/HIROMB-Based Marine Forecasts in Estonia: Problems, Experiences and Challenges.

Interest of using grid technology:

Why grid environment would be useful for application?	<i>Possibility to use computing resources to decrease computing time</i>
Current level of grid-enabling the application	<i>Prepared for usage in grid environment</i>
The foreseen issues to successfully port application on a distributed computing environment like the Baltic Grid infrastructure	<i>It would be reasonable to decrease the number of input and output files, because not all of them are necessary in each simulation.</i>

Contact person

Name	Petras Zemlys
Role in the team	leader
Institute/Company	Coastal Research and Planning Institute, Klaipeda University
E-mail address	petras.zemlys@ku.lt
Phone	+370 46 398881

3.2. TEXT-TO-SPEECH SERVICE

This interest group works on complex computation, which helps to solve prosody modelling problem for Lithuanian language. The users of such modeling procedures are located at Vilnius University, Kaunas University of Technology, Vilnius Pedagogical University. There will be some other users, after the first computing results will be achieved. The general description of the first application **DURMOD** prepared for usage in modelling:

- **Text-to-Speech in Grid.** Scientific domain of the application belongs to Text-to-Speech synthesis, requiring complex computations of phonemes durations modeling, based on “back-propagation” algorithm.
- **Text-to-Speech Analysis and Synthesis.** The goal of application is to extend and modify the computer synthesizer for English language as well as for Lithuanian language ("Aistis") and to implement the text-to-speech synthesis as Semantic Web application, operating in grid computing environment. The components of such development include phonema modelling for English and Lithuanian language, voice tone modelling and control, automatic text stressing, speech recognition elements, voice control, word clustering and morphological decomposition and some others.

Contact person:

Tomas Anbinderis, Vilnius University, Faculty of Mathematics and Informatics, 24 Naugarduko Str., Vilnius, ph.: +370 5 2193063, e-mail: tomas.anbinderis@mif.vu.lt

3.3. TEXT ANNOTATION SERVICE

This special interest group (SIG) is devoted to Computational Linguistics researchers, who are interested in using BalticGrid computational and dissemination resources. The users for the SIG are from Latvian University,

The following activities are currently related to this SIG:

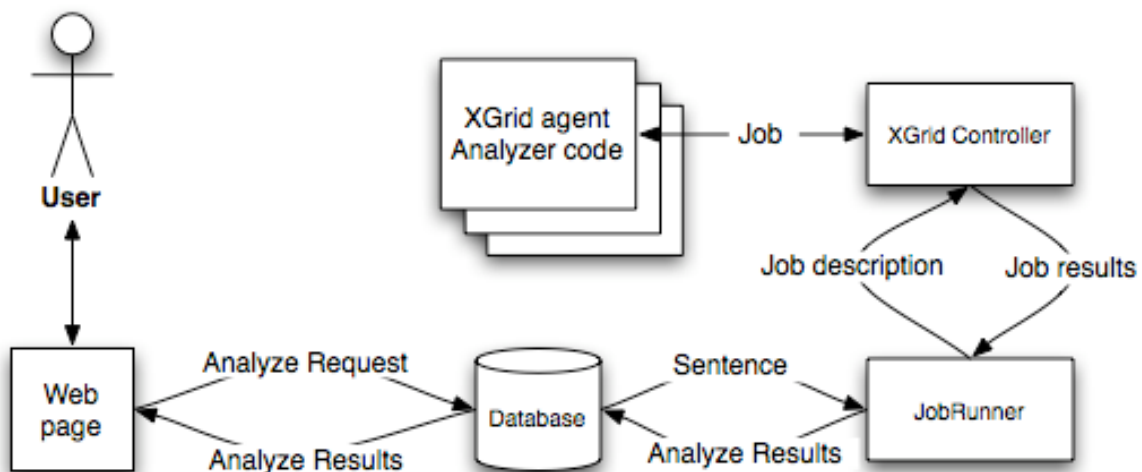
- [SentiKamols project](#) in University of Latvia is developing deep semantic parsing techniques for Latvian language. Besides basic grammar parsing for Latvian, the project utilizes techniques from Semantic Web and related formal logic-based approaches to enable formal reasoning about the facts mentioned in the text. One of the applications from this project has been successfully gridified in the Migrating Desktop environment of BalticGrid with the help of Poznan Super Computing Centre.
- [Lithuaninan online text corpus project](#) in Vytautas Magnus University (Kaunas) is developing a large and well ballanced text corpus with advanced online access interfaces.

Development of parallel text corpus of Lithuanian, Latvian and English has been initiated by [Faculty of Philology at Vilnius University](http://www.semanti-kamols.lv).

General description of the application *SemtiKamols*:

Scientific domain the application belongs to	<i>ontological linguistics</i>
Name of application	<i>SemtiKamols</i>
Web site of application	http://www.semanti-kamols.lv
<p><i>The goal of application is to ensure that ontologies both already established and ones created in Latvia are up to date and complete as possible for working with Latvian language. This first step would then allow to develop Semantic Web applications for working with Latvian language and interoperation with foreign languages. Things like analysis and synthesis of [a limited subset of] natural language constructs are a long term goal of this project, allowing development of other tools like quality translators and tools for formal text semantic proofing and annotation.</i></p>	

Architecture of application:



The components of the application are:

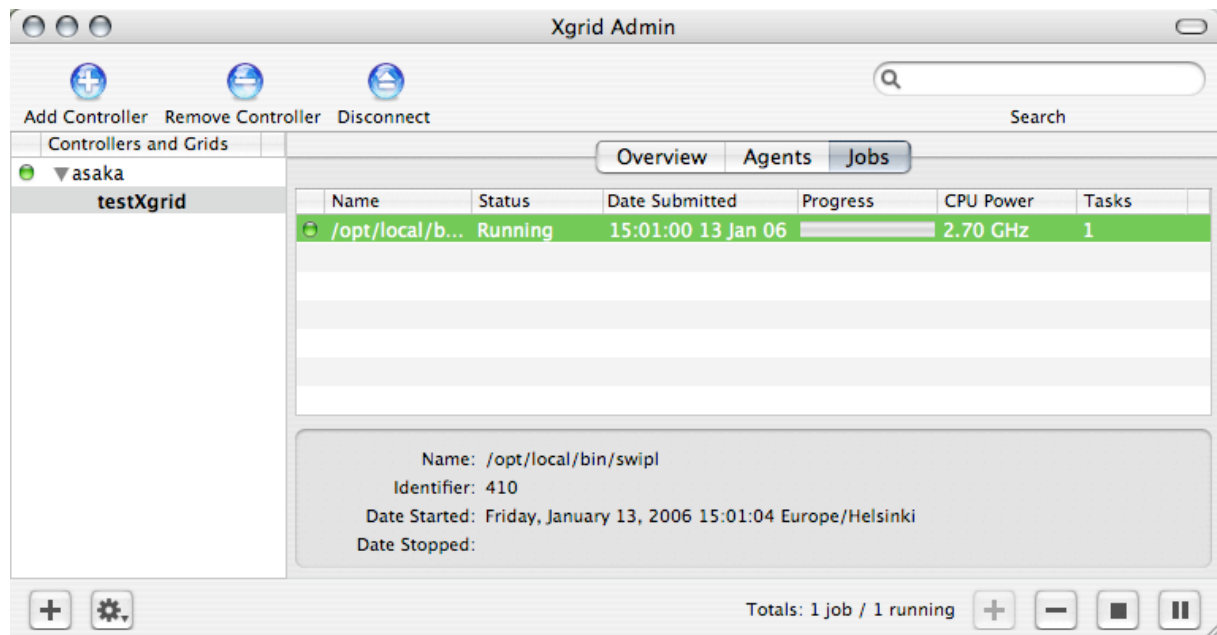
1. Web application, which places user requests for sentence processing into the database.
2. Database, where all analysis requests together with their results are stored.
3. Job runner, which polls database for new requests, and submits job requests to XGrid controller.
4. The jobs then are delegated to XGrid agents (worker nodes) where analyzer software is installed and invoked on job arrival.

5. Job results are also processed by XGrid, and delivered back to job runner.
6. Job runner receives job results and stores them into database so they are accessible to the web application.

Technology/paradigm that it uses:

The core analyzer application (written in Prolog) is computationally intensive. It performs extensive pattern matching and reasoning in the large-scale OWL DL ontology, which is converted into RDF format and stored in the RAM during analysis. Additionally, the application performs morphological and syntactic analysis based on lexical dictionary and production rules for word-form and context-free grammar matching. To optimize performance, the application generates large (~1Gbyte) amounts of RAM-stored intermediate results.

Currently the application itself is not distributed. To process large amounts of text or multiple simultaneous requests submitted via web, individual sentences are distributed for processing by multiple instances of the same application running on multiple XGrid servers in parallel.



Licensing issues:

Main license for the application	<i>Research project is part of the national program</i>
Third party commercial software	<i>SWI Prolog is licensed under GPL-2 and LGPL</i>
Describe the license under which your application can be distributed on the grid infrastructure	<i>NDA</i>

Usage:

Current level of usage (approximated number of jobs in month)	10000
Planned level of usage (approximated number of jobs in month, dates)	1000000
The plan of production in the next two years	<i>The new ontological linguistics analysis applications are under development. The goal is to apply these applications to the massive amounts of text, including those crawled from the web by the search engine. Unspecified large amount of computational power will be needed for that.</i>

Interest of using grid:

Why GRID environment would be useful for application?	<i>The jobs are easily parallelizable and there are lots of texts to process.</i>
Current level of grid-enabling the application	<i>Complete</i>
The foreseen issues to successfully port application on a distributed computing environment like the Baltic Grid infrastructure	<i>Will have to change code responsible for grid middleware invocation. There might be limited experience for porting Prolog applications in the Grid environment.</i>

Contact person:

Name	<i>Janis Dzerins</i>
Institute/Company	<i>IMCS LU</i>
E-mail address	<i>jonis@latnet.lv</i>
Phone	<i>+3719123913</i>

3.4. STELLAR SPECTRA SERVICE

The SIG is designed to serve researchers, mainly astronomers, involved in modelling of stellar and galactic chemical evolution. The research requires a theoretical interpretation of spectra and analysis of the main parameters of stellar atmospheres: temperature, pressure, chemical composition, age, etc. In order to obtain the most precise results it is important to make calculations using the atomic and molecular data arrays as large as possible with the most accurate atmospheric models. In a near future the Gaia Space Observatory will produce a huge amount of new spectral data, so there will be important to have powerful computing

resources. This Observatory is under construction by the European Space Agency. The astronomers of Vilnius University Institute of Theoretical Physics and Astronomy, as well as researchers from some other institutions participate actively in this project.

The prolongation of research may be done at nanoscale level:

The properties of nano-particles play a key role in technology and industry, ranging from the generation and distribution of electrical power to communication devices and the processing of information. The results of this research should be useful and attractive for a wide variety of users. However, the main aim of these investigations is Co nanoparticle and their optical and magnetic properties that are applied in the design of the information storage devices.

1. Develop and install a program for obtaining the optimal basis of relativistic wave functions by selecting the strongest mixing configurations. The program adopt to grid.
2. Develop and install a program for the cascade of radiative processes esmation.
3. Modeling and search of a morphology and electronic structure of the Co_{16} , Co_{18} , Co_{30} ir Co_{36} nano particles.
4. Equilibrium geometry search to obtain the most stable structures.
5. Optical spectra and magnetizability simulation of the investigated derivatives and comparison with experimental measurement.
6. Estimation of the abundance of Co in the stars of the Galaxy disk.
7. Examine the best condition for the problem management.
8. Installation of Dalton program to grid enviroment.

- General description of the application **SYNTSPEC**:

Scientific domain the application belongs to	<i>Astrophysics</i>
Name of application	<i>SYNTSPEC</i>
Goals of application	<i>Calculations of normalization to the continuum stellar spectra, that serves for determination of chemical composition of stars, their effective temperatures, surface gravity and turbulence motions in stellar atmospheres.</i>

Interest of using grid:

Why GRID environment would be useful for	<i>Possibility to run several jobs, make cascades,</i>
--	--

application?	<i>use big storage.</i>
Current level of grid-enabling the application	<i>Initial stage</i>
The foreseen issues to successfully port application on a distributed computing environment like the Baltic Grid infrastructure	<i>Distribute recourses is needed for the high quality results</i>

Contact person:

Name	<i>Grazina Tautvaisiene</i>
Role in the team	<i>Director, Chief Researcher</i>
Institute/Company	<i>VU TFAI</i>
E-mail address	<i>taut@itpa.lt</i>
Phone	<i>+37052610959</i>

- General description of the application **SMEFLUX**:

Scientific domain the application belongs to	<i>Astrophysics</i>
Name of application	<i>SMEFLUX</i>
Goals of application	<p><i>It is necessary to compute an absolute stellar energy fluxes, which are used for:</i></p> <ul style="list-style-type: none"> • <i>Investigations of main stellar atmospheric parameters</i> • <i>Spectral influence of chemical composition alterations to stellar spectra</i> • <i>Investigation of photometric methods of stellar parameter determinations (GAIA photometric system & Vilnius photometric system)</i>

Interest of using grid:

Why GRID environment would be useful for application?	<i>CPU resources, storage, RAM, possibility to run several jobs</i>
Current level of grid-enabling the application	<i>Initial stage</i>
The foreseen issues to successfully port application on a distributed computing	<i>Distribute recourses is needed for the high quality results</i>

environment like the Baltic Grid infrastructure

Contact person:

Name	<i>Sarunas Mykolaitis</i>
Role in the team	<i>researcher</i>
Institute/Company	<i>VU TFAI</i>
E-mail address	<i>sarunas@itpa.lt</i>
Phone	<i>+37052613440</i>

3.5. ATOMIC AND NUCLEAR COMPUTATIONS

The SIG unites research undertakings related to the investigation of structures at atomic and nuclear level. The users for this SIG are from Vilnius University, Institute of Theoretical Physics and Astronomy, Institute of Physics, some other institutions. It also has a potential to involve more users later, when the intermediate results will be achieved.

VPMS. The goal of the applications suggested is to setup of parallel scalable shell model code capable of effectively solving the problems of large dimensions (the matrix dimension $D \sim 1e8$). The main block of original program involves operation of a huge, non-homogeneously-sparse matrix on a vector, which is further normalized and orthogonalized to previous vectors. Pieces of vectors are distributed among nodes, and the matrix is computed on the fly. Different blocks of this matrix are assigned to different nodes, thus the final vector has to be gathered at storage nodes before orthogonalization. The module is developed applying C++ programming languages and using MPI, POSIX thread technologies. The spherical shell model proved to accurately describe low-excitation nuclear states as well as processes involving collective correlations (for example, deformations on Gamow-Teller excitations).

Name of application (software):	<i>VPSM</i>
Summary (a few paragraphs):	<i>A parallel, distributed-memory shell model code for large-scale nuclear structure calculations.</i> <i>Spherical shell model is used whenever accurate nuclear structure information is needed. Its applications range from explaining nuclear gamma-ray spectroscopy data to getting estimates for lepton-nucleus reaction rates in exploding stars. The success of the model is due to a good description of both the collective and the single-particle degrees of freedom. The model has its limitations. Since it</i>

	<p><i>takes into account all interactions between the valence particles in the chosen active orbits, larger nuclear systems require to diagonalize greater matrices. The dimension grows exponentially as the number of valence particles and/or active orbits increase. This leads to truncations with the loss of accuracy and difficulties of applying a more general theory in explaining the results.</i></p> <p><i>The code implements shell-model (with the core) paradigm on a distributed-memory computer network. The matrix is diagonalized using the Lanczos method, spectral functions are obtained using the method of moments. The code calculates energy spectra, Gamow-Teller distributions and selected observables. Among the planned extensions there is a calculation of weak-interaction matrix elements.</i></p>
Person responsible (names, contacts):	<i>Andrius Juodagalvis, Institute of Theoretical Physics and Astronomy, Vilnius, Lithuania</i>

ATOM. Objectives: 1) calculation of photon- and electron-impact excitation and ionization cross sections of atoms and ions and parameters describing polarization and angular distribution of fluorescence radiation and Auger electrons; 2) development of atom theory and its applications; 3) calculations of cascades in many-electron atoms. Several different program packages such as POLARIZ, AS, GLOCHAS have been used.

General description of the application **ATOM**:

Scientific domain the application belongs to	<i>Atomic Physics</i>
Name of application	<i>Atomic spectra</i>
Goals of application	<i>Development of atom theory and it's applications</i>
Architecture of application	<i>Solution of integro-differential equation, variational procedures, diagonalization of large matrix, tensor algebra.</i>

Interest of using grid:

Why GRID environment would be useful for application?	<i>Need of the large RAM</i>
---	------------------------------

Contact person:

Name	<i>Pavel Bogdanovich</i>
Role in the team	<i>leader</i>
Institute/Company	<i>ITPA</i>
E-mail address	<i>pavlas@itpa.lt</i>
Phone	<i>+37052620949</i>

3.6. COMPUTATIONAL MODELLING OF HETEROGENEOUS PROCESSES

Applications described below present mathematical/computational models and simulation procedures for different aspects of material science in areas mentioned in the title:

CellMembrane:

Name of application (software):	<i>Electric Conduction in Cell Membrane</i>
Summary (a few paragraphs):	<i>This program solves the electric conduction in cell membrane, calculates the electrical characteristics of photolipidic thin membrane with tiny hole. Applications: understanding of Alzheimer's disease, Parkinson's disease and others neurodegenerative diseases.</i>
Person responsible (names, contacts):	<i>Tadas Meskauskas tadas.meskauskas@mif.vu.lt</i>

FrontMove:

Name of application (software):	<i>Solution of the front movement</i>
Summary (a few paragraphs):	<i>This program solves the Front movement in the bistable system, calculates the front movement speed, front relaxation time. The main principle was to change the Cauchy for the nonlinear differential equation with the boundary problem with by the boundary value depending on time.</i>
Person responsible (names, contacts):	<i>Antanas Raguotis araguotis@hotmail.com</i>

Scatter Solver

Name of application (software):	<i>scatter_solver</i>
Summary (a few paragraphs):	<i>Scatter solver is custom C++ application, designed to perform computer simulation of light wave 2D propagation in scattering linear and non-linear media. It employs finite differences method for solution of non-linear Schrödinger equation with stochastic term, thus demands high computing power.</i>
License agreement:	<i>GNU GPL</i>
Person responsible (names, contacts):	<i>Mantas Puida (e-mail mantasp@gmail.com)</i>

Shgsolve:

Name of application (software):	<i>shgsolve</i>
Summary (a few paragraphs):	<i>Application applies a finite difference method for solving a system of nonlinear Schroedinger equations in the cylindrical coordinates. It is used for the modelling of short laser pulses in nonlinear environments.</i>
Person responsible (names, contacts):	<i>dr. Andrius Kurtinaitis, andrius.kurtinaitis@maf.vu.lt</i>
Names of persons using this application:	<i>dr. Andrius Kurtinaitis, prof. Aleksandr Dementjev</i>

LOAD:

Scientific domain the application belongs to	<i>Scientific domain the application belongs to: Material sciences, electrochemistry</i>
Name of application	<i>Numerical calculation of the distribution of loaded particles</i>
Goals of application	<i>Mathematical simulation of diffusion processes of loaded particles in various media including electrochemical cells. The application can be used to calculate bipolar electro dialysis in environmentally clean technologies, treatment of salt-water effluent etc. An original computation method is used for the appropriate calculations.</i>
Architecture of application	<i>The components of the application are:</i>

<i>The application consists of input module, calculation module, and output module.</i>

Licensing issues:

Main license for the application	<i>Research project is founded by national founds</i>
----------------------------------	---

Interest of using grid:

Why GRID environment would be useful for application?	<i>The jobs can be computed independently and their number is crucial for understanding the processes to be simulated</i>
Current level of grid-enabling the application	<i>The application is being prepared for gridization.</i>

Contact person:

Name	<i>Bruno Martuzans</i>
Role in the team	<i>Scientific supervisor</i>
Institute/Company	<i>IMCS LU</i>
E-mail address	<i>bruno@latnet.lv</i>
Phone	<i>+371 7085832</i>

4. CONCLUSIONS

The activity NA3 identifies applications and their communities for the Baltic Grid and develops support for them. Application Special Interests Groups are to be formed as a framework for developing new successful BG user communities. The target for SIGs is to establish at least two SIGs per Baltic State with at least 12 active members per group.

The BalticGrid's deliverable DNA3.6 presents the results achieved by implementing project's milestones:

- MNA3.2 (Technical specification of Special Interest Groups) - to define and develop topics and technical specification for Special Interest Groups;
- MNA3.3 (Application support road map and Identification of support staff) - to arrange content and plan for support of applications by expert groups and by provision of useful tools;
- MNA3.4 (Application Areas for SIG identified);
- MNA3.12 (SIGs operational) – partly.

The contextual and technical specification of the Special Interest Groups leads to a definition of an organizational, operational and computing environment, suitable to select topics for SIGs as application disciplines. According to the targets of BG, topics like “Baltic Sea Ecosystem Modelling”, “Text Annotation Service”, “Text-to-Speech Service”, “Atomic and Nuclear Computations”, “Stellar Spectra Computations”, “Computational Modelling of heterogeneous Processes” fit well to the BG project objectives and will be considered in future analysis, description and deployment.