



MIGRATING DESKTOP INSTALLATION AND INTEGRATION OF APPLICATIONS

Report on MD Installation and Integration of Applications

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Abstract: This deliverable describes the current status of integration of Migrating Desktop Platform for applications within BalticGrid infrastructure. The Migrating Desktop has been deployed within BalticGrid infrastructure and successfully integrated with several applications, implemented or “gridified”. In everyday work MD proved its usefulness as a tool that makes grid application usage much easier and more intuitive which is essential for the encouraging potential beneficiaries to reach profits from using grid infrastructure for compute- and data-intensive applications.

The important goal for the months to come is the integration of next applications that are progressively deployed within BalticGrid infrastructure.





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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 large-scale success of information technologies and the demand for ones, especially such as computing, data mining, and visualization depend essentially on how easy is the access to these technologies by users that are non-experts in the technologies and systems being used. It is also crucial to enable user-friendly and intuitive access to grid environment to speed better deployment of projects within new scientific user communities. To achieve this goal the Migrating Desktop system has been chosen as a general-kind tool for accessing and managing the project applications, tools, resources and services. MD represents advanced graphical user interface and a set of tools combined with a user-friendly outlook, similar to window based operating systems.

1.1 PURPOSE OF THE DOCUMENT

The purpose of this document is to present the results of conceptual and technical analysis done for Migrating Desktop, while reaching milestones MNA3.1 (Technical analysis of applications in HEP, MS, BI). The purpose of this document is to present the current status of integration of Migrating Desktop Platform with BalticGrid infrastructure and applications.

1.2 ABBREVIATIONS

BG – Baltic Grid
BI – Bioinformatics
HEP – High-Energy Physics
MD – Migrating Desktop
MS – Material Sciences

2 EXECUTIVE SUMMARY

The activity NA3 reported in this document aims to present the current status of implementation of Migrating Desktop Platform within BalticGrid infrastructure and integration of MD for applications.

The Migrating Desktop Platform is a powerful and flexible user interface to Grid resources that gives a transparent user work environment and easy access to resources and network file systems independently of the system version and hardware. It allows the user to run applications and tools, manage data files, and store personal settings independently of the location or the terminal type.

An overview of Migrating Desktop Platform, its features and role within the BalticGrid project as a general character tool for accessing and managing the project resources and services has been shortly presented. The Migrating Desktop Platform was enhanced to ensure compatibility with BalticGrid environment and successfully deployed within project infrastructure. The deployment procedures and installations available for grid users and application developers are described. This document summarizes possibilities and technical aspects of integration of BalticGrid applications within Migrating Desktop Platform. The integration of pilot applications: GAMESS and SentiKamols, chosen to be integrated within Migrating Desktop Framework to prove correctness of integration mechanisms and procedures, is described. The last chapter summarizes and points out the future plans concerning Migrating Desktop.

Migrating Desktop has been deployed within BalticGrid infrastructure and successfully integrated with several applications, implemented or “gridified” within BG project. In everyday work MD proved its usefulness as a tool that makes grid application usage much easier and more intuitive which is essential for the encouraging potential beneficiaries to reap profits from using grid infrastructure for compute- and data-intensive applications.

The important goal for the coming activities in BalticGrid with respect to MD is the integration with next applications that are progressively deployed within BalticGrid infrastructure.

3 SHORT OVERVIEW OF THE MIGRATING DESKTOP PLATFORM

The Migrating Desktop Platform is a powerful and flexible user interface to Grid resources that gives a transparent user work environment and easy access to resources and network file systems independently of the system version and hardware. It allows the user to run applications and tools, manage data files, and store personal settings independently of the location or the terminal type.



Fig. 1. Migrating Desktop main window

The Migrating Desktop (MD) is an advanced graphical user interface similar to a window-based operating system that hides the complexity of the grid middleware and makes access to the grid resources easy and transparent. The Migrating Desktop offers:

- a flexible personalized working environment available independently of the user location, scalability and portability,
- a set of tools,
- a single sign-on mechanism,
- support for multiple grid infrastructure and special support for „roaming users”

so that they can use their personalized working environment regardless of their physical location and used operating system.

The Migrating Desktop strictly cooperates with the Remote Access Server (RAS), which intermediates between different grid middleware and applications. RAS offers a well-defined set of web-services that can be used as an interface for accessing HPC systems and services (based on various technologies) in a common, standardized way. The Roaming Access Server consists of several independent modules responsible for job submission, job monitoring, user

profile management, data management, authorization, and application information management.

Open architecture of the Migrating Desktop Platform makes integration with various tools, applications and middleware quite easy (in contrast to other products that are only Globus-oriented in most cases). Such approach allows increasing functionality in an easy way without the need of architecture changes.

Migrating Desktop was created in the EU project CrossGrid (IST-2001-32243, <http://www.crossgrid.org>) and is currently developed in the EU project Interactive European Grid (contract no. 031857, <http://www.interactive-grid.eu/>), where the functionality of Migrating Desktop for handling interactive grid applications (i.e. grid applications characterized by the interaction with a person in a processing loop) is being implemented.

4 INSTALLATION WITHIN BALTICGRID INFRASTRUCTURE

4.1 INTEGRATION WITH BALTICGRID INFRASTRUCTURE

One of the first steps performed within NA3 activity of BalticGrid project, were changes in Migrating Desktop platform components to be fully compatible with project testbed. This was a base for extending (“tuning-up”) Migrating Desktop general functionality to fulfill requirements of BalticGrid applications and communities. The Migrating Desktop Platform is currently developed only within int.eu.grid - the EU Interactive European Grid Project (development of functionality related to handling interactive jobs), however all changes made within BalticGrid project are also added to product releases.

4.2 INSTALATION PROCEDURE

The software produced within int.eu.grid is released periodically and carefully tested during the validation process. Modules that passed the validation are available in int.eu.grid project repository (<https://wiki.fzk.de/i2g/index.php/Repositories>) as a set of RPM binary packages, which can be installed using "rpm" tool available in RedHat distribution. The Migrating Desktop and Roaming Access Server are “independent” products and could be distributed separately.

The RAS package consists of 4 parts:

- Roaming Access Server - i2g-ras-server-*.noarch.rpm
- RAS LDAP database - i2g-ras-ldap-*.noarch.rpm
- RAS MYSQL database - i2g-ras-mysql-*.noarch.rpm
- Job Submission Service - i2g-ras-jss-*.noarch.rpm

The MD package consists of single file:

- MD client - i2g-md-client-*.noarch.rpm

To standardize installation process and to make it easier to site administrators installation user guide has been prepared and published on desktop home pages (<http://desktop.psnc.pl>). This document describes requirements, installation process and configuration issues.

4.3 DEPLOYMENT IN BALTICGRID TESTBED

Migrating Desktop has been deployed within BalticGrid infrastructure and is being successfully used by project community for accessing project resources and handling applications supporting the entire job life-time (jobs defining, submission of jobs to BG testbed, monitoring execution and visualisation of result).

There are few Migrating Desktop Platform installations in BalticGrid testbed:

- “Development” installations – used for development and testing of new features – deployed in PSNC (e.g. on servers cedrus.man.poznan.pl, balsa.man.poznan.pl) and VU (e.g. md.grid.vtu.lt);
- “Production” installation – used by users and application developers – deployed as one of BalticGrid core services (ras.balticgrid.org);
- Document describes deployment of MD servers;
- MD clients are also available, however not directly from default html page.

This document is intended only to show current status. All documents necessary to understand MD/RAS architecture are available on MD home pages: <http://desktop.psnk.pl>

5 INTEGRATION WITH BALTICGRID APPLICATIONS

The key feature of the Migrating Desktop is the possibility of easy adding various tools, applications and support visualisation of different formats. Due to the complex nature of grid applications and unpredictability of their requirements, the Migrating Desktop offers a framework that can be easily extended on the basis of a set of well-defined plug-ins used for: accessing tools, defining job parameters, pre-processing job parameters before submission, and visualisation of job results. It makes that product significantly more flexible than specialized tools (e.g. portals) designed only for a specific application.

5.1 INTEGRATION PROCEDURES

Requirements of BalticGrid applications were collected and analysed at the early stage of the project. The analysis resulted in design of integration procedures and classification of applications regarding to features required by graphical interface for grid operations. The performed analysis gave also important feedback to the developers concerning identification requirements that are not supported by current version of the Migrating Desktop. The conclusions were described in project deliverable DNA3.2-“Procedures for integration of application with Migrating Desktop”. This document provides description of possibilities and technical aspects of integration of the Migrating Desktop with applications concerning their requirements of graphical interface as well as integration procedures.

Applications that requirements are accomplished by MD functionality can be integrated without any additional effort. In other cases application developers have to add extra functionality to fulfil application’s specific needs using concept of plug-ins as integration points between the Migrating Desktop and applications.

Depending on the functionality that the developer would like to add to the Migrating Desktop framework, he/she has to choose what kind of plug-in has to be implemented. The developer can choose from the types described in this document:

- Job input plug-in – for defining specific job input parameters;
- Job process plug-in – if any additional activities should be performed before submitting a job (e.g. job parameters have to be optimized before submission);
- File viewer plug-in – if applications produce non-standard format files that are not handled by the Migrating Desktop and that have to be presented in a user-friendly graphical format;
- Application viewer plug-in – for the visualisation of job results that are produced as a set of files or that have to be pre-processed (e.g. any animations, visualisation of meteorological data as weather forecast map, etc.)
- Tool plug-in – for adding any Java tools to the Migrating Desktop framework;

5.2 INTEGRATED PILOT APPLICATIONS

The BalticGrid applications are dedicated to wide spectrum of various disciplines of science such as:

- bioinformatics - which requires sharing data from many sources and a diverse set of tools.
- material science - including atomic and molecular structures, modelling of advanced technological materials,
- high-energy physics - including statistical data analysis, production of Monte Carlo samples and distributed data analysis, nuclear and sub-nuclear physics and multi-body problems
- linguistic applications

GAMESS and SentiKamols applications were chosen to be integrated within Migrating Desktop Framework as a pilot applications to prove correctness of integration mechanisms and procedures.

5.2.1 GAMESS

Application description

GAMESS is a program for ab initio molecular quantum chemistry. Briefly, GAMESS can compute SCF wave functions ranging from RHF, ROHF, UHF, GVB, and MCSCF. Correlation corrections to these SCF wave functions include Configuration Interaction, second order Perturbation Theory, and Coupled-Cluster approaches, as well as the Density Functional Theory approximation. Nuclear gradients are available, for automatic geometry optimization, transition state searches, or reaction path following. Computation of the energy hessian permits prediction of vibrational frequencies, with IR or Raman intensities. Solvent effects may be modelled by the discrete Effective Fragment Potentials, or continuum models such as the Polarizable Continuum Model. Numerous relativistic computations are available, including third order Douglas-Kroll scalar corrections, and various spin-orbit coupling options. The Fragment Molecular Orbital method permits use of many of these sophisticated treatments to be used on very large systems, by dividing the computation into small fragments.



Fig. 2 GAMESS application – job submission plug-in.

Integration within Migrating Desktop Framework

Integration of GAMESS application within Migrating Desktop Framework includes:

- implementation of specific plug-ins for job defining to make job submission easier and more intuitive for the user (see
- Fig. 2)
- adapting of open-source JMol application as Migrating Desktop plug-in for visualization of application results (see Fig. 3).
- preparation and publishing for BalticGrid users community a user guide describing in details procedure of definition, monitoring and results visualisation of GAMESS application .

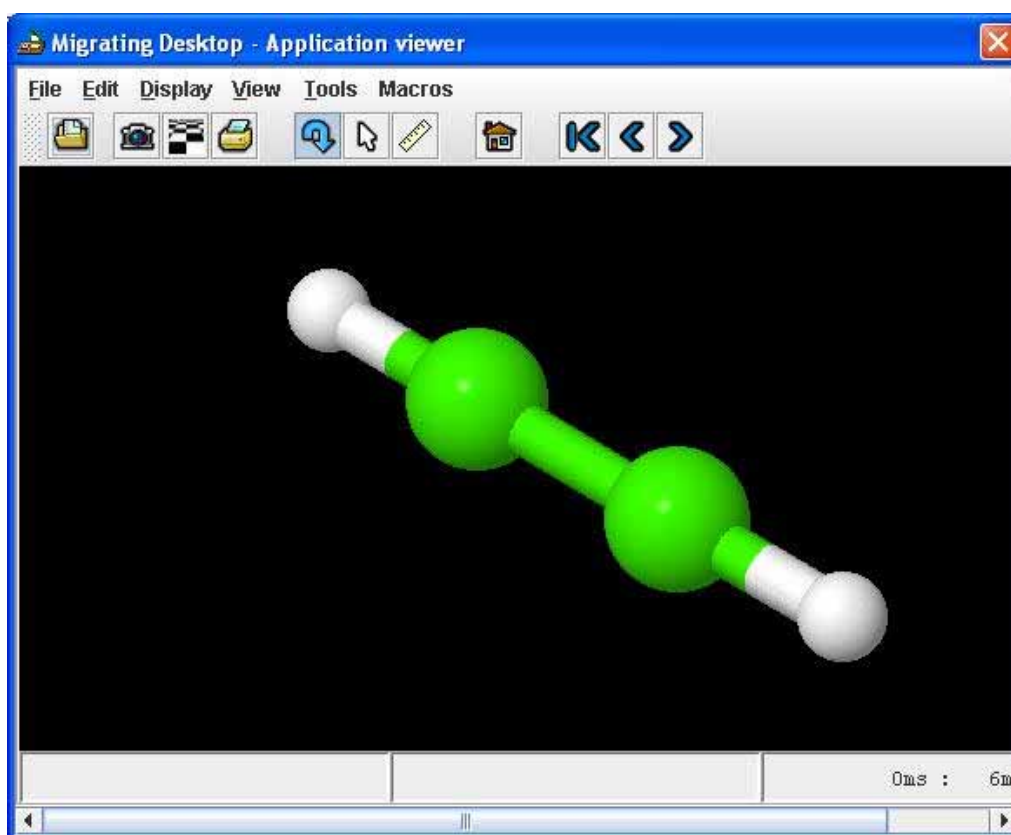


Fig. 3 GAMESS application – job visualization plug-in.

5.2.2 SentiKamols - Natural Language Processing

Application description

SentiKamols project in University of Latvia aims to develop semantic resources and methodologies for automatic meaning extraction from Latvian texts. This ultimate goal requires the lower levels of the language analysis, namely, morphology, syntax and lexical semantics, to be properly implemented in the first place. 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. The advantage of such semantic framework is that it avoids the text disambiguation problem at the lower parsing levels, and leaves it to the higher semantic processing layers. The semantic processing layer is being built upon techniques adapted from the frame semantics (FrameNet), ontologies (OntoSem, SUMO) and ACE (Attempto Controlled English).



Fig. 4 SentiKamols application – job submission plug-in.

Integration within Migrating Desktop Framework

Work performed to integrate SentiKamols application encompasses:

- implementation of specific job submission plug-in (see Fig. 4)
- preparing job visualization plug-in that use system default web-browser for visualization of HTML page containing application results (see Fig. 5).
- preparation and publishing for BalticGrid users community a user guide describing in details procedure of definition, monitoring and results visualisation of SentiKamols application .

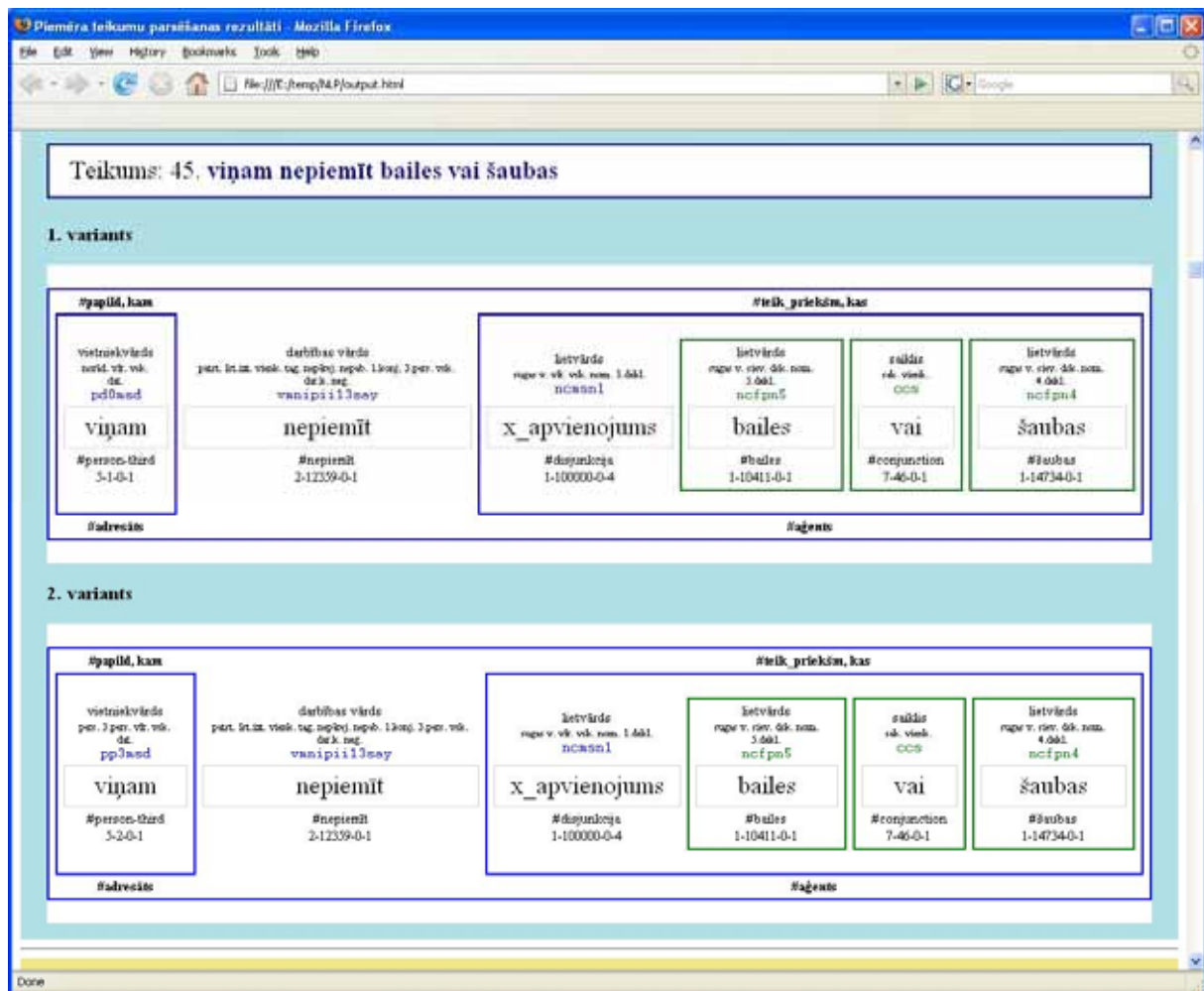


Fig. 5 SentiKamols application – job visualization plug-in.

6 CONCLUSIONS AND FUTURE PLANS

Migrating Desktop has been deployed within BalticGrid infrastructure and successfully integrated with several applications, implemented or “gridified” within BG project. In everyday work MD proved its usefulness as a tool that makes grid application usage much easier and more intuitive which is essential for the encouraging potential beneficiaries to reap profits from using grid infrastructure for compute- and data-intensive applications.

The most important goal for the coming months is the integration of remaining applications which are progressively deployed within BalticGrid infrastructure. There are few requirements that are important from application point of view, which are not supported by current Migrating Desktop version. Based on detailed analysis and cooperation with application developers, extension to existing functionality will be gradually designed and deployed. Another task is the enhancement of Migrating Desktop Platform components to follow the rapid development of grid standards and services for ensuring compatibility with BalticGrid testbed in terms of the jobs submission, running and monitoring processes’ state.