Computing and Informatics, Vol. 32, 2013, 1100–1115

NEW SCIENCE GATEWAYS FOR ADVANCED COMPUTING SIMULATIONS AND VISUALIZATION USING VINE TOOLKIT IN PL-GRID

Piotr Dziubecki, Piotr Grabowski
Michał Krysiński, Tomasz Kuczynski, Krzysztof Kurowski
Tomasz Piontek, Dawid Szejnfeld

Poznan Supercomputing and Networking Center
Noskowskiego 12/14, 61-704, Poznan, Poland
e-mail: {deepres, piotrg, mich, docentt, krzysztof.kurowski, piontek, dejw}@man.poznan.pl

Abstract. A Science Gateway is a connection between scientists and their computational tools in the form of web portal. It creates a space for communities, collaboration and data sharing and visualization in a comprehensive and efficient manner. The main purpose of such a solution is to allow users to access the computational resources, process and analyze their data and get the results in a uniform and user friendly way. In this paper we propose a complex solution based on the Rich Internet Application (RIA) approach consisting of a web portal powered by Vine Toolkit with Adobe Flex/BlazeDs technologies. There are two Science Gateways described in detail one for engineers to manage computationally intensive workflows used in advanced airplane construction simulations, and one for nanotechnology scientists to manage experiments in nano-science field calculated with Density Functional Theory (DFT). In both cases the results show how modern web solution can help scientists in their work.

Keywords: Science gateway, Web2.0, ABINIT, Vine Toolkit, Liferay, workflow, Adobe Flex, material science, nanotechnology

Mathematics Subject Classification 2010: 68-XX

1 INTRODUCTION

Advanced web-based graphic and multimedia oriented user interfaces (GUIs) designed for scientists and engineers could change the way users collaborate, share computing experiments, data and work together to solve day-to-day problems. Moreover, future science and engineering gateways will influence the way users will access not only their data, but also control and monitor their demanding computing simulations using the Internet. To allow users to interact remotely with future supercomputers and large-scale computing environments in a more interactive and visual manner we present a tool called Vine Toolkit that has been successfully used as a core web platform for various gateways [1, 2]. Vine Toolkit is a modular, extensible and easy-to-use tool as well as high-level Application Programming Interface (API) for various applications, visualization components and building blocks to allow interoperability between many different HPC and grid technologies. It supports Adobe Flex and BlazeDS technologies to allow developers to create advanced, rich web applications similar to many stand-alone GUIs [3]. Additionally, Vine Toolkit has been integrated with well-known open source web frameworks such as Liferay and Gridsphere. In this paper, we briefly describe new technological solutions relevant for advanced scientific and engineering portals driven by example scientific and engineering needs.

1.1 Related Work

Currently, there are several grid portal frameworks available that help users to create advanced and easy-to-use science gateways. P-GRADE is a good example of highly integrated parallel application development web-based system for Grid and clusters [4]. It uses Globus, Condor-G, ARC, BOINC and MPICH-G2 as grid-aware middleware to conduct computations. Another example is a collaborative environment where scientists can safely publish their workflows and experiment plans, share them with groups and find those of others, called `myExperiment.org` [5]. In this approach, workflows, other digital objects and bundles (called Packs) can now be swapped, sorted and searched like photos and videos on the Web. Unlike Facebook or MySpace, myExperiment fully understands the needs of the researcher and makes it really easy for the next generation of scientists to contribute to a pool of scientific methods, build communities and form relationships – reducing time-to experiment, sharing expertise and avoiding reinvention. EnginFrame is a good example of a web-based front-end for simple job submission, tracking and integrated data management for HPC applications and other services [6]. EnginFrame can be easily plugged on several different schedulers or grid middlewares like Platform LSF, Sun Grid Engine, PBS, or gLite middleware. Another approach to build an API that provides the basic functionality required to build distributed applications, tools and frameworks is SAGA [7] – it offers however only easy to use programming interface without any GUI support needed to create easy-to-use science gateway. Yet, another approach to build similar to Science Gateway solution is one of problem solving environments:

GridSpace2 [8, 9]. GridSpace2 is a novel virtual laboratory framework enabling researchers to conduct virtual experiments on Grid-based resources and other HPC infrastructures. GridSpace2 facilitates exploratory development of experiments by means of scripts which can be expressed in a number of popular languages, including Ruby, Python and Perl. The framework supplies a repository of gems enabling scripts to interface low-level resources such as PBS queues, EGEE computing elements, LFC directories and other types of Grid resources. Moreover, GridSpace2 provides a Web 2.0-based Experiment Workbench supporting joint development and execution of virtual experiments by groups of collaborating scientists. GridSpace2 main idea to enable HPC environments via web interface is very similar to Vine Toolkit main idea, however GridSpace with its scripts is more like programming environment for the Grid – suitable for advanced users or programmers; on the other hand, Vine Toolkit Applications do not require from the user knowledge of scripting languages and focus on delivering ready to use GUIs. Moreover, thanks to Vine Toolkit native JSDL and BES support (both OGF standards [10]), the QosCosGrid middleware stack used in the prototype portal can be easily changed to any type supported by Vine middlewares without changes in code or even the need to restart the portal. To the best of our knowledge Vine Toolkit is the most generic and advanced web-based framework integrated with Adobe Flex technology available.

1.2 Scientific Objectives

In this paper we present two portal solutions which cover different goals regarding the use of HPC infrastructure. The first solution is the Flowify portal. The gateway itself was built for engineers from the EADS group during the wow2green (Workflows On Web2.0 for GRid Enabled infrastructures in complex Enterprises) BEinGRID business experiment project. The main goal in this project was to build a web-based platform using grid solutions to manage computationally intensive workflows used in advanced airplane construction simulations by engineers in different geographically distributed enterprise departments. Flowify helps users synchronize the data processing for execution and collection of results in an automated fashion. Easy-to-use Flowify workflow interfaces are provided as intuitive web applications or integrated with commonly used tools. Thus, many users can dynamically and simultaneously form workspaces, share not only data for their computing experiments but also manage the whole process of advanced computations. An important goal was to tighten the co-work of geographically dispersed company departments to solve advanced and very sophisticated computational problems.

The second example is the Nano-Science Gateway which has been created for nanotechnology science. One of the main goals of this portal is to combine experimental nano-scale measurements, real data analysis and verifications, together with advanced modeling and numerical simulations on supercomputers based on collaboration between scientists in this multidisciplinary research field. Nanoscientists require efficient and accurate scientific applications on supercomputers with a supporting infrastructure that allows them to focus on the research domain without knowledge of the technically complicated IT systems. Thus, we had to prepare a user friendly, domain-focused science gateway which allows users to solve nanotechnology-related problems in an intuitive way. The proposed solution was the web-based collaborative platform based on Vine Toolkit and Liferay, along with web-based tools integrated with grid services and the scientific applications like ABINIT, Quantum Espresso, NAMD. Basic functionality covers such stages as preparation of input data, submission of jobs, monitoring and controlling simulations, post processing and analysis of the outcomes, data storage and archiving. Other advantages of the integrated environment include automation of additional actions like data movement, data conversion, data post processing and visualization.

In both cases the list of scientific objectives is related to development of the whole gateway and specific web application. Different containers are used: GridSphere for Flowify and Liferay for Nano-Science Gateway, different middlewares and different applications; Vine Toolkit is the common part in both Gateway solutions.

2 DESCRIPTION OF THE PROBLEM SOLUTION

Next three paragraphs present how the scientific objectives were handled regarding developed portal solutions. The "Software used" section explains Vine Toolkit architecture and history of improvements, then in last two subsections the problem solution for both Gateways: Flowify and Nano-Science Gateway is described.

2.1 Software Used

Starting from the top of the Vine Toolkit software stack, it provides an efficient and robust user interface framework based on the Adobe Flex and BlazeDs software. Vine allows the integration of the rich internet application standard directly to a browser and enables applications to act and look exactly as their stand-alone versions. Thus, it is possible to create advanced portal applications like science gateways where developers can create web-based versions of many legacy applications and their GUIs. One of the key new requirements for Vine Toolkit regarding the integration with existing portal frameworks was to enable web application developers to create rich and advanced user interfaces as quickly as possible. Initially, we tried to use JS/AJAX-based frameworks within Vine Toolkit. Various problems related to the software portability in different web browsers encouraged us to migrate to other frameworks for the development and deployment of cross-platform rich Internet applications. Eventually, Adobe Flex was chosen for developing rich and advanced user interfaces in Vine Toolkit. The main reason was that at the time of the project inception, Microsoft Silverlight was far behind Flex in terms of functionality [11]. Also, the licensing favored Flex which is open source. Obviously, the presentation layer is a front end to various components and services provided by Vine Toolkit, but it is getting ever more important once advanced web applications are available. Thanks to a pluggable Vine architecture it is possible to extend its base functionality in a uniform way. For instance, at the beginning Vine Toolkit offered only a support for the Globus Toolkit middleware. Currently, it is possible to use the majority of leading middleware stacks: GRIA, gLite, UNICORE, QosCos middleware and many other well-known standards, such as OGF JSDL, OGF OGSA-BES or OGF-HPC Profile [12]. Technically speaking, a new service in Vine can be added by creating a separate project and implementing a set of predefined APIs. Then, after a proper configuration, it can be used transparently by the end user without any additional changes in the application code. Finally, Vine offers various deployment configurations including standalone mode, web service mode and more importantly a ready to use integration with portal environments and portlet containers, e.g. Gridsphere or Liferay [14, 15]. Therefore, with a single software stack it is possible to build a complex solution consisting of services, a portal and a set of user-customized applications available at once as a web gateway. Vine was designed to work with well-known JSR-168 open standard and its reference implementation and Tomcat web application container [16]. Since version 1.1, Vine Toolkit also supports Liferay JSR-286 enterprise portal [17]. Consequently, Vine Toolkit gives its users a great opportunity for creating and delivering production-quality web environments as it covers major web-based development aspects, especially for scientific and computing portals.

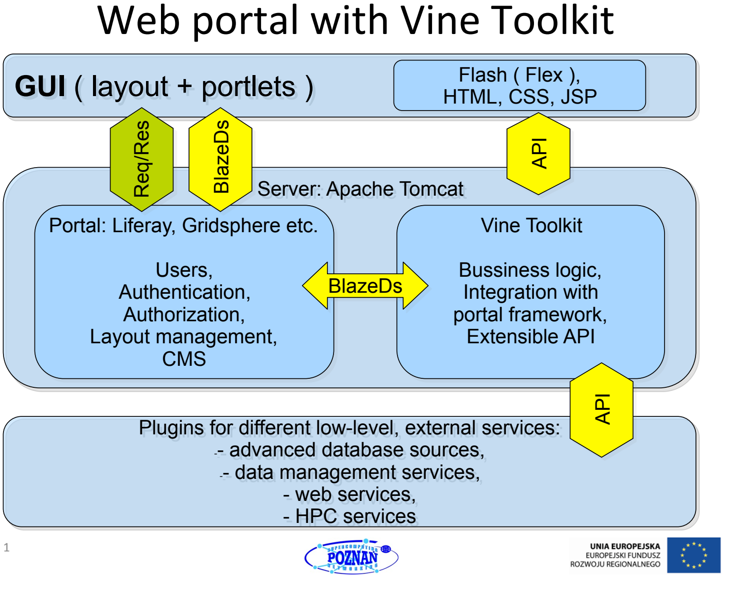

Figure 1. Portal with Vine Toolkit generic schema

2.2 Flowify Portal

One of the main component is a built-in grid level meta-scheduling broker service called GRMS which allows IT administrators to apply various resource management policies, in particular load balancing of jobs submitting to computing clusters and data centers to meet peak demands. As a core workflow engine within the Flowify gateway we used the Kepler/Ptolemy standalone application/framework according to requirements for workflow support and description collected from engineers. Please note that the pluggable architecture of Vine Toolkit allows developers to add other workflow management systems. The graphical user web interface for workflow management and control was created with Adobe Flex technology to provide easy-to-use and very similar interface to the stand-alone Kepler application. Thanks to Flowify capabilities, workflow creators are able to share workflow definitions with other users via the Internet. Computing simulations and generated data can be shared among different groups of users supporting inter and intra department co-operation within given company. At the same time users have a fully transparent access to underlying computing resources, so they can focus on research goals using domain specific interfaces and completely ignore the complexity of the underlying IT infrastructure.

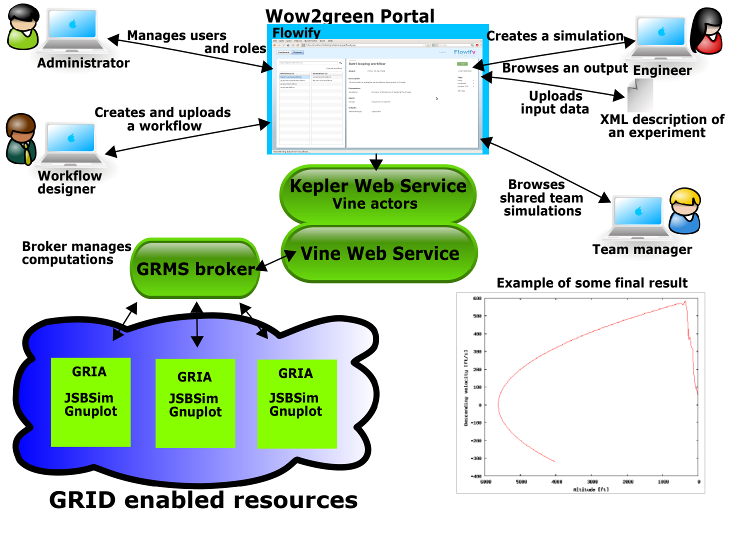

Figure 2. Flowify portal components, actors and results

Beside Vine Toolkit and GridSphere portal framework Flowify architecture consists of several components: Vine web service – web service that exposes a subset of functionality to external systems/services related to the grid middleware abstraction; Kepler workflow engine – core part of the Kepler/Ptolemy standalone application/framework for workflow management; Kepler engine web service – web service that exposes the workflow engine functionality to external systems/services; set of Kepler Vine actors – base components of the workflow, where jobs will be submitted through the vine web service to allow grid-independent actions on resources; GRMS broker with web service interface – job broker component with advanced scheduling methodology to balance resource usage in the grid environment; GRIA middleware – grid middleware – service-oriented infrastructure (SOI) designed to support B2B collaborations through service provision across organizational boundaries (it could be exchanged as the grid access is abstracted through the Vine Toolkit usage); GRIA Information Web Service – web service that exposes the information about available GRIA resources and also about queues' statistics in the batch systems behind the GRIA services.

Flowify web application is the main end user web interface at the portal level. The welcome screen consists of the so called Dashboard which summarizes the simulations runs in the grid resources. End user is able to see the simulations' current statuses with links leading to the given simulation details. The other part of the web interface is a browser with two panels – the left side is a workflow and simulation search place, the right side shows the details of the selected element. In case of the workflow template user is able to specify input parameters and files and later start a new simulation of it. Details of the workflow template present the overall description and the description of all parameters, it is also possible to view the graphical representation of the chosen workflow. In case of parameter form, a simple parameter sweep is possible by defining a set of values, for example for the given run. The possibility to tag the elements like workflow or simulation and later search for any object with the given tag value assigned is an important feature. Beside simple status information after the simulation start, user can also see advanced history of the simulation. The history shows a list of all applications executions, which are part of the workflow on the grid resources including such information like start and end time or DNS host name. Flowify portal allows specifying a group of users and defining share policies at the portal and grid resources level. It was important due to direct downloads of results accordingly to the end users privileges set at the portal level – in this case functionality of the GRIA middleware regarding groups and roles was used intensively. Four end users types are distinguished from the conceptual point of view: administrators, workflow designers, engineers and team managers. Through built-in role management system different kind of users have different rights and responsibilities in the complex organizational company structure.

2.3 Nano-Science Gateway

The most advanced part of this nanotechnology science gateway is ABINIT portal client. The ABINIT simulation software package allows users to solve problems such as finding the total energy, charge density and electronic structure of systems made of electrons and nuclei within Density Functional Theory (DFT), using pseudopotentials and a planewave basis [18, 19]. ABINIT also includes options to optimize the geometry according to the DFT forces and stresses, or to perform molecular dynamics simulations using these forces, or to generate dynamical matrices, Born effective charges, and dielectric tensors. Excited states can be computed within the Time-Dependent Density Functional Theory (for molecules), or within Many-Body Perturbation Theory. Despite of its usefulness in computations, being a command-line tool, ABINIT requires from the user not only domain-specific knowledge but also some computer science related accomplishments and ABINIT in/out data structures familiarity. In order to hide the complexity and provide a web-based collaborative access to ABINIT, we created many new rich web applications using Vine Toolkit and Adobe Flex. Consequently, we are able to support the transparent web access to sequential and parallel execution of DFT codes deployed on HPC computing clusters available for users in the PL-Grid infrastructure. By providing basic and advanced modes we are able to support both experts and beginners during their simulation studies. Continuous meetings with end users were a great opportunity to gather new requirements, e.g. tools to parse input/output parameters in the form-like panel for ABINIT and other DFT code, e.g. Quantum Espresso. Some parameters that were not reflected in the parameter input form could be easily added now using a new rich editor in the advanced mode. It should be noted that inputs needed for ABINIT job submission are pseudopotential files. Using the built-in Vine Toolkit file manager users can easily access, copy and assign appropriate files. It is also possible to store users' files by taking the advantage of Vine Toolkit files repository as well as advanced access control mechanisms to share them according to defined policies.

After preparing a set of parameters and selecting steering parameters for DFT calculations, a user can add another set of parameters to be solved in parallel. When the whole experiment is ready (typically, it consists of several parameter sets) the user can send the experiment to a Grid middleware controlling remote computing clusters. In this approach, we used the QosCosGrid middleware stack together with a metascheduler services called Grid Resource Management System (GRMS). Therefore, we were able to make the underlying HPC resources fully transparent for end-users, so they could focus only on domain-specific interfaces and problems instead of struggling with computing infrastructure details, such as available processing power, deployed libraries or memory limits. After job submission the user can monitor all his/her simulations by simply checking the progress bars. Additional monitoring tool is a chart presenting the relative difference between subsequent computation iterations. If the user notes that the difference does not converge during experiment, he/she may decide to cancel this task in order to save the computational power. It is also possible to cancel the whole experiment – in this case all pending tasks (for corresponding parameter sets) are cancelled. Immediately after each job completion, the user can see generated results in the portal. As it was mentioned above, all the ABINIT output files are stored in a Vine repository or can be transferred to remote file servers, e.g. GridFTP or more advanced Data Management Services, e.g. iRODS or DMS. The calculated functions of the total density of electronic states (DOS) line charts can also be displayed as visualization results. It is possible to view multiple series from different tasks on the same chart. The chart can be dynamically cropped and zoomed and special values like the Fermi energy can be also marked on the chart (if it was calculated in given case). For those applications we used Vine extensions based on Adobe Flex. Figure 3 shows the example experiment and its visualization results.

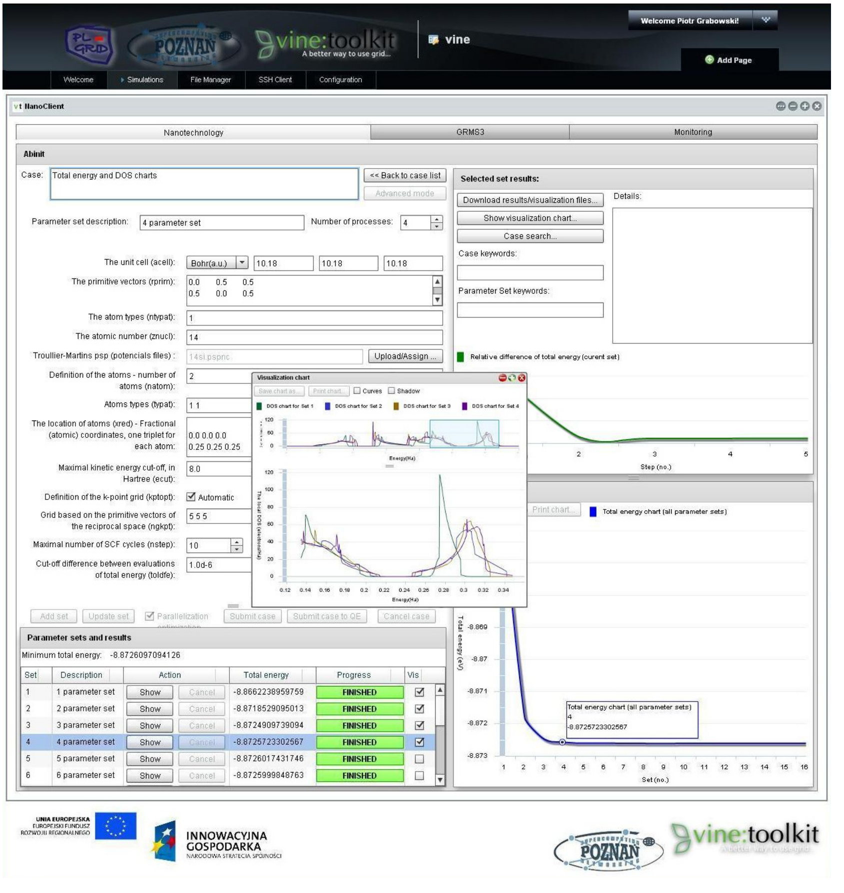

Figure 3. Nano-Science Gateway – ABINIT web client: Total energy calculation and calculated functions of the total density of electronic states (DOS) line charts

All parameter sets and corresponding computing jobs together with their results are stored as cases for further use. This allows users to start or re-submit long-term calculations from the portal, observe their progress after some time (possibly with another browser and session), view the results of completed experiments and reuse the previous experiments altering some parameters. To enable quick search of a certain example all parameter sets and previous cases can be annotated with keywords by users. Thus, it is possible to look for similar experiments descriptions and results using these tags by other users working on similar data sets. In this case, a special module for web searching is used with two data sources available: Google and ScienceDirect. The Nano-Science Gateway also allows for viewing computing resources and monitoring their characteristics to provide a useful feedback for end users, developers and administrators in different administrative domains where computing clusters or other HPC resources are located. In order to gather all presented metrics, various monitoring tests are invoked periodically and their results are presented as graphical maps or diagrams in the portal using Adobe Flex applications. For example, thanks to the QosCosGrid middleware, results of bi-directional tests of cross-domain QCG-OMPI and QCG-ProActive applications measuring bandwidth and latency between clusters located in different administrative domains can be visualised [20]. One of the most useful features of this part of the portal are Gantt charts showing local and cross-domain job executions as well as advance reservation and co-allocation of computing resources in time. Both monitoring tools are presented in Figure 4.

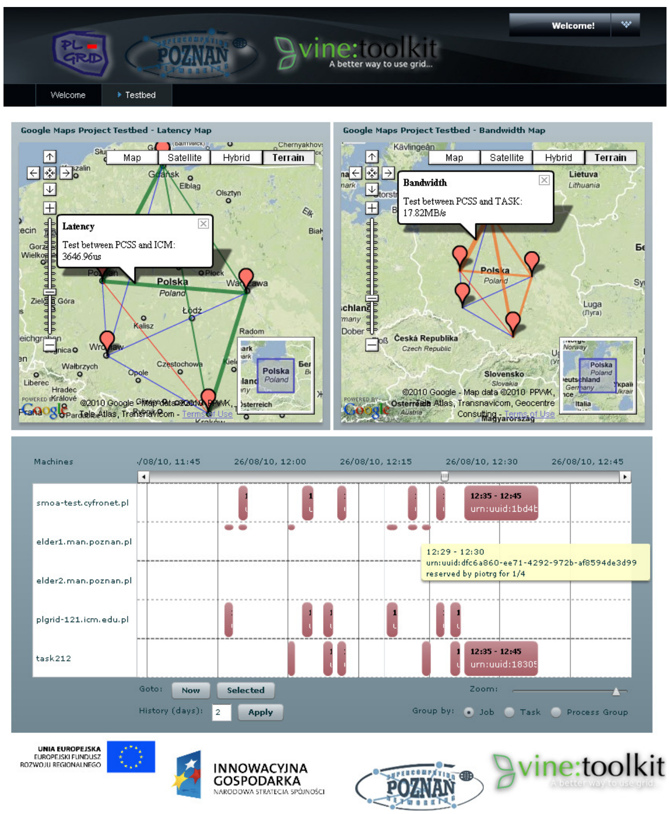

Figure 4. Nano-Science Gateway – Testbed information page showing network latency and bandwidth together with active advance reservations in HPC clusters available in the PL-Grid infrastructure

3 RESULTS

The presented Flowify portal system solves many problems in a complicated grid environment. It reduces the response time of the grid system through brokering and automatic resource management, causes better usage of distributed grid resources as resource broker, balances their usage, reduces errors during the overall process of advanced simulations as the workflows are provided and validated by the experienced workflow designers, simplifies administration efforts in large scale computing environments by the simple and easy to use web interface and finally provides user friendly process of preparing and managing workflow simulations. The second solution allows end users to focus only on nano-science and abstract their scientific research work from the IT environment they have to use. Graphical interfaces plus support for native input files for applications like ABINIT make the work easier and more productive. Users have access to full history of scientific outcomes and previous applications runs so next simulation could be based on the previous ones. Modifications and experiment repetitions are more user friendly, many actions are automated (such as data management). Users can download output data at any time and place and do further analysis locally if desired. What is important, Nano-Science Gateway was successfully presented at the NANO 2010 workshop co-located with the 4^{th} National Conference on Nanotechnology [21]. During the workshop scientists could test our new portal solution solving on-line ABINIT tutorial examples on the real HPC testbed without the need to access remote computing clusters using SSH or file transfer protocols. Users were using web browsers to perform all the computing simulations on remote machines.

4 CONCLUSIONS AND FUTURE WORK

In this paper, we briefly presented our approach to build Science Gateways using our Vine Toolkit integrated with the Adobe Flex software development kit. The presented web-based gateway supports various nanotechnology scientists in execution and management of large-scale simulations on computational grids using DFT code like ABINIT or Quantum Espresso. The described framework offers an effective way to start, monitor and control scientific applications via web based user-friendly graphical interfaces. Other Vine Toolkit based gateways were successfully developed and adopted in several other communities and R & D projects like QosCosGrid, BEinGrid, Omii-Europe or HPC-Europa mentioning Flowify solution. Currently Vine Toolkit is being enhanced and tested under the national Polish Grid Infrastructure (PL-Grid) project and is planned to be deployed in production environments. Future works on the Vine Toolkit based Science Gateways is divided into two parts: various extensions to the existing ABINIT, Quantum Esspreso, NAMD clients and support for another applications and packages like MOPAC. Many existing users identified several new applications that can be added to the gateway easily, e.g. NWChem or BLAST/CLUSTALW2, and their integration will be a next step. Then, we would like to extend the gateway to support all major applications used for large-scale parallel simulation in nanotechnology and molecular chemistry/biology, thus giving scientists the possibility to make their advanced calculations in one collaborative web space. Some additional features will be added to incorporate popular social networking capabilities; some of them are currently available in Vine Toolkit and Liferay repositories. Social networking features will be used to improve data sharing and semantic descriptions of the performed experiments and obtained results.

Acknowledgements

The authors would like to thank all people whose work allowed us to provide the Nano-Science Gateway for the scientific community and Flowify Portal for EADS. Special thanks go to Mr. Michal Hermanowicz and people at the Institute of Physics, Poznan University of Technology who provided a lot of useful feedback to user interfaces and generated main requirements. This work has been funded by the PL-Grid project (contract number: POIG.02.03.00-00-007/08-00, website: `www.plgrid.pl`) [22]. The PL-Grid project is co-funded by the European Regional Development Fund as part of the Innovative Economy program. The Flowify Portal was built for "wow2green" Business Experiment 23 of BEinGrid EU integrated FP6 project (CN: 034702, `www.beingrid.eu`) [23].

REFERENCES

[1] Russell, M.—Dziubecki, P.—Grabowski, P.—Krysinski, M.—Kuczynski, T.—Szejnfeld, D.—Tarnawczyk, D.—Wolniewicz, M.—Nabrzyski, J.: The Vine Toolkit: A Java Framework for Developing Grid Applications. Parallel Processing and Applied Mathematics 2008, Lecture Notes in Computer Science No. 4967, pp. 331–340.

[2] Szejnfeld, D.—Dziubecki, P.—Kopta, P.—Krysinski, M.—Kuczynski, T.—Kurowski, K.—Ludwiczak, B.—Piontek, T.—Tarnawczyk, D.—Wolniewicz, M.—Domagalski, P.—Nabrzyski, J.—Witkowski, K.: Vine Toolkit – Towards Portal Based Production Solutions for Scientific and Engineering Communities with Grid-Enabled Resources Support. Scalable Computing: Practice and Experience, Vol. 11, 2011, No. 2, pp. 161–172.

[3] Adobe, Flex/BlazeDs, `http://www.adobe.com/products/flex/`.

[4] P-GRADE, `http://www.p-grade.hu/`.

[5] myExperiment, `http://www.myexperiment.org/`.

[6] EnginFrame, `http://www.nice-software.com/web/nice/products/enginframe`.

[7] SAGA, `http://saga.cct.lsu.edu/`.

[8] Gubała, T.—Bubak, M.: GridSpace – Semantic Programming Environment for the Grid. 6^{th} International Conference on Parallel Processing and Applied Mathematics (PPAM 2005), LNCS 3911, 2006, pp. 172–179.

[9] Bubak, M.—Bali, B.—Bartyski, T.—Ciepiela, E.—Funika, W.—Gubała, T.—Harlak, D.— Kasztelnik, M.—Kocot, J.—Malawski, M.—

Meizner, J.—Nowakowski, P.—Rycerz, K.: Capabilities of Grid Space Virtual Laboratory. In Proceedings of the Cracow Grid Workshop, Krakow (Poland) 2010.

[10] OGF, http://ogf.org/.

[11] Microsoft, Silverlight, http://www.silverlight.net/.

[12] Kurowski, K.—Piontek, T.—Kopta, P.—Mamoski, M.—Bosak, B.: Parallel Large Scale Simulations in the PL-Grid Environment. Computational Methods in Science And Technology, Special Issue 2010, pp. 47–56.

[13] Kurowski, K.—de Back, W.—Dubitzky, W.—Gulys, L.—Kampis, G.—Mamonski, M.—Szemes, G.—Swain, M.: Complex System Simulations with QosCosGrid. Lecture Notes in Computer Science, Vol. 5544, 2009, pp. 387–396, DOI: 10.1007/978-3-642-01970-8 38.

[14] Gridsphere, http://www.gridsphere.org/.

[15] Liferay, http://www.liferay.com/.

[16] JSR-168, http://jcp.org/en/jsr/detail?id=168.

[17] JSR-286, http://jcp.org/en/jsr/detail?id=286.

[18] Gonze, X.—Amadon, B.—Anglade, P.-M.—Beuken, J.-M.—Bottin, F.—Boulanger, P.—Bruneval, F.—Caliste, D.—Caracas, R.—Cote, M.—Deutsch, T.—Genovese, L.—Ghosez, Ph.—Giantomassi, M.—Goedecker, S.—Hamann, D.R.—Hermet, P.—Jollet, F.—Jomard, G.—Leroux, S.—Mancini, M.—Mazevet, S.—Oliveira, M. J. T.—Onida, G.—Pouillon, Y.—Rangel, T.—Rignanese, G.-M.—Sangalli, D.—Shaltaf, R.—Torrent, M.—Verstraete, M. J.—Zerah, G.—Zwanziger, J. W.: ABINIT: First-Principles Approach of Materials and Nanosystem Properties. Computer Phys. Commun. 180, pp. 2582–2615, 2009.

[19] Gonze, X.—Rignanese, G.-M.—Verstraete, M.—Beuken, J.-M.—Pouillon, Y.—Caracas, R.—Jollet, F.—Torrent, M.—Zerah, G.—Mikami, M.—Ghosez, Ph.—Veithen, M.—Raty, J.-Y.—Olevano, V.—Bruneval, F.—Reining, L.—Godby, R.—Onida, G.—Hamann, D. R.—Allan, D. C.: A Brief Introduction to the ABINIT Software Package. Zeit. Kristallogr. 220, pp. 558–562, 2005.

[20] Agullo, E.—Coti, C.—Herault, T.—Langou, J.—Peyronnet, S.—Rezmerita, A.—Cappello, F.—Dongarra, J.: QCG-OMPI: MPI Applications on Grids. Future Generation Computer Systems, Vol. 27, No. 4, pp. 357–369, ISSN 0167-739X. DOI: 10.1016/j.future.2010.11.015.

[21] The 4th National Conference on Nanotechnology, http://www.nano2010.put.poznan.pl/.

[22] PL-Grid Project, http://www.plgrid.pl/en.

[23] BEinGrid Project, http://www.beingrid.eu/.

Piotr Dziubecki received his M. Sc. degree in Computer Science from Czestochowa University of Technology in 2006. The same year he joined Poznan Supercomputing and Networking Centre, Poland where he works as a software analyst. Before joining PSNC he was involved in the development and benchmarking of the parallel multiple sequence alignment software. Currently his main area of interest is interface design for gridaware portals. Since 2006, until now Piotr has participated in a number of EU funded projects such as inteliGrid, OMII-Europe, and BeInGrid. He is an author or co-author of several papers in professional journals and conference proceedings.

Piotr Grabowski obtained his M. Sc. in Computer Science in 1998 at Poznań University of Technology, Distributed Computer Systems. After his M. Sc., he joined the programmers group at PUT and worked on mobile network protocol analyzers software for Siemens A. G. and Tektronix, Inc. Since 2002 he has been working in Poznań Supercomputing And Networking Center, Application Department. In 2002 he joined GridLab project and worked on access for mobile users. Since 2005, until now he has participated in a number of EU funded projects such as inteliGrid, OMII-Europe, and BeInGrid and local initiatives on enabling access from Mobile Devices and Portal technologies. The main thrust of his current research work are Mobile Devices and e-Mobility, Web Services and Web technology. He is an author or co-author of several papers in professional journals and conference proceedings. Since 2010 he leads User Interface Laboratory at PSNC.

Michał Krysiński received his M. Sc. degree in Computer Science from Poznań University of Technology in 2008. Since 2006, when he joined PSNC, he has participated in a number of EU funded projects such as OMII-Europe, and ACGT. He is an author or co-author of several papers in professional journals and conference proceedings.

Tomasz Kuczynski holds M. Sc. Eng. degree in Computer Science (Software Engineering) from Czestochowa University of Technology. Since 2004 employed at PSNC. He was involved in many, both EU-funded and national research projects, such as GridLab, HPC-Europa, OMII-Europe, BEinGRID, ACGT to name a few. Led users' interface WP in the ClusterIX national project. Contributed to the GridSphere portal project. Currently he is taking part in PL-Grid national project. Main areas of expertise are web technologies and security. He is credited with discovery of numerous security vulnerabilities in portal software including Liferay, Apache Tomcat, Mortbay Jetty, Caucho Resin and others. All vulnerabilities discovered by Tomasz was verified and published by the US-CERT (Department of Homeland Security of the USA).

Krzysztof Kurowski holds the Ph. D. degree in Computer Science and he is leading now Applications Department at Poznan Supercomputing and Networking Center, Poland. He was involved in many EU-funded R & D projects in the following areas Distributed and High Performance Computing and Grids over the last few years, such as GridLab, inteliGrid, HPC-Europa, or QosCosGrid. He was a research visitor at University of Queensland, Argonne National Lab, and CCT/Louisiana University. His research activities are focused on the modeling of advanced applications, scheduling and resource management in networked environments. Results of his research efforts have been successfully presented at many international conferences and workshops. The work has been funded by the HPC-Europa2 project under grant agreement number 228398, website: `www.hpc-europa.org`.

Tomasz Piontek received his M. Sc. in computer science in 1998 from Poznań University of Technology (Parallel and Distributed Computing). 1998–2002 he worked at Poznań University of Technology as a member of the programmers group worked on mobile network protocol analyzers software for Siemens A. G. and Tektronix, Inc. Since 2002 he has been working in Poznań Supercomputing And Networking Center in Application De-partment and was involved in many EU-funded and national R & D projects in the area of Grids: GridLab, ACGT, QosCosGrid, PL-Grid, MAPPER. His research interests include distributed computing, large-scale simulations and resource management. Since 2010 he leads the Large-scale Simulations Laboratory at PSNC.

Dawid Szejnfeld is Head of Laboratory of Portal Applications of Application Department at PSNC. He received his M. Sc. in Computer Science from Poznań University of Technology in 2001. After studies he gains commercial experience during his work for ALMA S. A. and for one of the biggest commercial web portals in Poland called Wirtualna Polska. Since 2004 as PSNC employee he has been involved in many EU funded projects in the area of web and grid technologies and web security like HPC-Europa, OMII-Europe, BEinGRID. Currently involved in HPC-Europa2 project and polish infrastructural project called PL-Grid. He is an author or co-author of several papers in professional journals and conference proceedings. Technical certification gained: MCP, MCSE and MCDBA.