Online Web-Based Science Gateway for Nanotechnology Research

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

Poznań Supercomputing and Networking Center, Poznań, Poland
{deepres,piotrg,mich,docentt,krzysztof.kurowski,
piontek,dejw}@man.poznan.pl
http://www.man.poznan.pl

Abstract. The main objective of Science Gateways is to give users remote access to supercomputers and large-scale computing environments in an interactive, web-based and graphical manner. We present a tool, called Vine Toolkit, that has been successfully used as a core web platform for various Science Gateways. Vine Toolkit is a modular, extensible and easy-to-use tool as well as a high-level Application Programming Interface (API) for various applications, visualization components and building blocks. In a nutshell, it allows interoperability between many different HPC and grid technologies within the service layer. As a result, Vine Toolkit provides an ability to build a portal upon different HPC technologies working together to deliver a complete solution to the users. In this article, we briefly describe our most complex and feature-rich project – the Nanotechnology Gateway, as well as a set of tools relevant to advanced scientific portals, development of which was driven by various requirements defined by scientists and gathered in scope of the PL-Grid project.

Keywords: Science Gateway, Web2.0, ABINIT, Vine Toolkit, Liferay, Java, Adobe Flex, Material Science, Nanotechnology.

1 Introduction

Advanced web-based graphic- and multimedia-oriented user interfaces (GUIs) designed for scientists and engineers could change the way their users collaborate, share computing experiments and data, and work together to solve day-to-day problems. Moreover, the future science and engineering gateways influence not only the way the users access their data, but also how they control and monitor their demanding computing simulations. In order to allow users to communicate remotely with supercomputers and large-scale computing environments in a more interactive and graphical manner, we present a tool, called Vine Toolkit, that has been already successfully used as a core web platform for various Science Gateways [1], [2], [3]. Vine Toolkit is a modular, extensible and easy-to-use Java-based tool as well as high-level Application Programming Interface (API) for

M. Bubak, T. Szepieniec, and K. Wiatr (Eds.): PL-Grid 2011, LNCS 7136, pp. 205–216, 2012.
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various applications, visualization components and building blocks. In this way, it allows interoperability between many different HPC and grid technologies. Below, we present a list of modules and plugins currently provided by Vine Toolkit as well as standards supported by this tool:

- job submission and monitoring: QosCosGrid 2.0 [4], [5], UNICORE 6 [6], gLite3 [7], GRIA 5.3 [8], Globus Toolkit 4.0.x, 4.2.1 [9],
- data access and management: IRODS [10], Storage Resource Broker, Storage Resource Manager [11], OGSA-DAI 2.2 [12],
- supported standards and services: BES [13], JSDL [14], RUS [15], Active Directory [16].

Moreover, Vine Toolkit supports also Adobe FLEX and BlazeDS technologies, allowing developers to create rich and advanced web applications similar to many stand-alone Graphical User Interfaces. Additionally, the tool has been integrated with well-known open source web frameworks such as Liferay and Gridsphere [17]. In this chapter, we briefly describe new technological solutions relevant to advanced scientific and engineering portals. Their development was driven by various requirements defined by scientists and gathered in scope of the PL-Grid project.

The rest of this chapter is organized as follows. In Section 2, related work in area of Science Gateways and Science Gateway frameworks is presented. Section 3 briefly describes our main motivations. Then, in Section 4, there are short descriptions of Scientific Applications developed with use of the described solution. Finally, Section 5 contains information about the planned future work.

2 Related Work

Currently, there are several approaches to implementing the Science Gateway concept. There is a group of frameworks facilitating design and creation of Science Gateways as well as already running portals ready to be used by the scientists. Among available tools that help users to create advanced science gateways, P-GRADE is a good example of a parallel application development system for Grid and clusters [18]. It uses Globus, Condor-G, ARC, BOINC and MPICH-G2 as grid-aware middleware to conduct computations. EnginFrame is another good example of a web-based front-end for simple job submission, tracking and integrated data management for HPC applications and other services [19]. EnginFrame can be easily plugged to several different schedulers or grid middlewares like: Platform LSF, Sun Grid Engine, PBS, or gLite. A slightly different approach to an API that provides basic functionality required to build distributed applications is presented by SAGA [20]. It focuses on delivering a set of programming interfaces covering the functionality of an HPC-aware application. Unfortunately it does not provide a GUI support, needed to create an easy-to-use Science Gateway (see the Vine Toolkit and SAGA comparison Table 1).

Fortunately, apart from development environments, there are also several sites offering direct access to specialist applications for scientists. A good example

Table 1. SAGA vs Vine Toolkit comparison

Middleware	**Vine Toolkit**	**SAGA – Java adaptors**
gLite 3 – Cream	Yes	Yes – JSAGA
gLite 3 – WMS	Yes	Yes – JSAGA
gLite 3 – JDL	Yes	under development – JSAGA
Globus Toolkit	Yes (4.0.x, 4.2.1)	Yes – JSAGA/JavaGAT
Globus Toolkit – MyProxy	Yes	Yes – JSAGA
Globus Toolkit – gsiftp	Yes	Yes – JSAGA
Globus Toolkit – WS-GRAM	Yes	Yes – JSAGA
BES	Yes	Yes – JSAGA
JSDL	Yes	Yes – JSAGA
GRIA	Yes (5.3)	No
UNICORE 6	Yes	Yes – JSAGA
Active Directory	Yes	No
Java Keystore	Yes	Yes – JSAGA
X509 Certificates	Yes	Yes – JSAGA
Storage Resource Manager	Yes	Yes – JSAGA
Storage Resource Broker	Yes	Yes – JSAGA
(S)FTP, SSH, HTTP(S), ZIP	Partly (http, SSH applet)	Yes – JSAGA/JavaGAT
local data management	Yes	Yes – JSAGA
WebDav	Yes	No
VOMS	Yes	Yes – JSAGA
iRODS	Yes	Yes – JSAGA
NAREGI (Super Scheduler)	NO	Yes – JSAGA
OGSA-DAI	Yes (2.2)	No
RUS	Yes	No
QosCosGrid	Yes	No
GRMS,GRMS3	Yes	No

of such well-established Science Gateway is `nanohub.org` [21]. Its main purpose is to deliver tools and materials, as well as to help with education, research and collaboration in nanotechnology. According to statistics provided by `nanohub.org`, they have over 10,000 simulation users and over 50,000 interactive users. This is a result of a wide range of nanotechnology applications and simulations/visualizations available within the portal. Regarding technical details, the `nanohub.org` web interface serves as a proxy between a remotely installed application and the end user. In order to achieve that, a Java applet with VNC plugin is used to connect the user to the remote GUI of the desired application.

Another example of a collaborative environment where scientists can safely publish their workflows and experiment plans, share them with groups and find those published by other users, is `myExperiment.org` [22]. In this approach, workflows, other digital objects and bundles (called Packs) can be swapped, sorted and searched like photos or videos on the Web. Unlike Facebook or MySpace, myExperiment fully understands the needs of the researchers; making it really easy for the next generation of scientists to contribute to a pool of scientific methods, build communities and form relationships. In this way, it reduces the time needed to experiment and to share expertise, as well as helps to avoid

reinvention. At last, we should not forget about similar projects – GridSpace [32] and InSilicoLab [31], that have been developed in the frame of PL-Grid.

The aforementioned examples differ from each other in implementation and visual form, still all of them were designed to solve specific scientific problems.

3 Motivation

Since its planning stage, one of the main goals of the Science Gateway for nanotechnology was to combine experimental nano-scale measurements, real data analysis and verification together with advanced modeling and numerical simulations on the PL-Grid computing resources. According to our analysis, based on the user feedback from the "Vine-users" mailing list [30] and surveys conducted at the `vinetoolkit.org` website, many researchers need efficient and easy-to-use interfaces to their scientific applications. However, they do not have a need for understanding of the underlying middleware services and IT systems. Therefore, we decided to develop a user-friendly, domain-focused Science Gateway that allows scientists to solve, run and control nanotechnology simulations in an intuitive way. The proposed solution is a web-based collaborative platform, that takes advantage of Vine Toolkit and Liferay, along with web-based tools integrated with QosCosGrid middleware [4], [5]. Additionally, scientific applications like ABINIT and Quantum Espresso are supported. The basic mode of the gateway use covers many functionalities, such as: preparation of input data, submission of jobs, monitoring and controlling simulations, post-processing and analysis of their outcomes, data storage and archiving [23]. In advanced mode, users can benefit from additional actions, like data migration, conversion, post-processing and visualization.

4 Scientific Applications

The most advanced part of our Science Gateway for nanotechnology research consists of two web-based interfaces for scientific applications: ABINIT and Quantum Espresso [24], [25].

The ABINIT simulation software package allows users to solve problems like finding the total energy, charge density and electronic structure of systems made of electrons and nuclei within Density Functional Theory (DFT), using pseudopotentials and planewave basis. ABINIT also includes options to optimize a geometry according to the DFT forces and stresses, and to perform molecular dynamics simulations using these forces, as well as to generate dynamical matrices, Born effective charges, and dielectric tensors. Excited states can be computed within Time-Dependent Density Functional Theory (for molecules) or within Many-Body Perturbation Theory. However, ABINIT itself defines several requirements towards the user:

– the user needs to know how to translate domain-specific problem to an ABINIT task;

- the command-line tool requires from the user experience with ABINIT in/out data structures;
- in case of parallel or large scale deployment, the user has to be familiar with many complex IT and HPC technologies.

In order to hide this complexity, we successfully developed a web-based collaborative interface enabling access to ABINIT, with use of Vine Toolkit and Adobe Flex [26]. Consequently, we are able to support fully transparent web-based access to sequential and parallel ABINIT executions deployed on computing clusters within the PL-Grid infrastructure. The list below contains the main features of our web interface:

- basic and advanced modes provide support both for experts and beginners;
- instead of using SSH, file transfer protocols, or other tools, the users can manage even complex simulation and data operations using web browsers;
- several tools facilitating the process of data visualization and analysis.

In addition, to meet specific users requirements, we developed web-based tools which provide means to analyze input/output parameters in a form-like panel – for ABINIT and other DFT code, e.g. Quantum Espresso. In this way, some of the parameters that were not reflected in the parameter input form can be easily added using a new rich editor of the interface advanced mode. One should note, that the inputs required for ABINIT job submission are pseudopotentials files. Using another web-based tool – Vine Toolkit File Manager – the users can easily access, copy and assign appropriate files stored on remote machines. What is even more important, the user is able to visualize data in the Science Gateway immediately after the simulation is completed. The calculated functions of the total density of electronic states (DOS) can be easily displayed as visualization results. It is also possible to view multiple series from different simulations on the same chart. The chart can be dynamically cropped and zoomed. What is more, special values like the Fermi energy can be marked on the chart. The example layout of the basic mode for calculation of total energy using ABINIT is presented in Fig. 1. The example case consists of 16 parallel executions of ABINIT using MPI processes on four cores. Fig. 1 shows also sample charts generated after ABINIT simulations. Moreover, in case of band structure calculations all required post-processing procedures are realized in the background, and only a final picture containing band structure chart is shown to the users. An additional, useful component is the Nano Structure Builder graphical tool, which allows to create and edit 3D crystallographic super cells and to generate ABINIT-compatible descriptions. Therefore, the users are able to prepare the whole simulation within the Science Gateway, without the need to use third party software. Nano Structure Builder is a web-based application that provides functionalities available in both commercial and open source tools, such as XCrysDen or GoVasp [27], [28]. XCrysDen is an open source application that enables visualizations of crystalline and molecular structures. GoVasp is a commercial software providing, i.a., a structure builder – a graphical tool that enables creation and manipulation of solid state structures. Currently, Nano

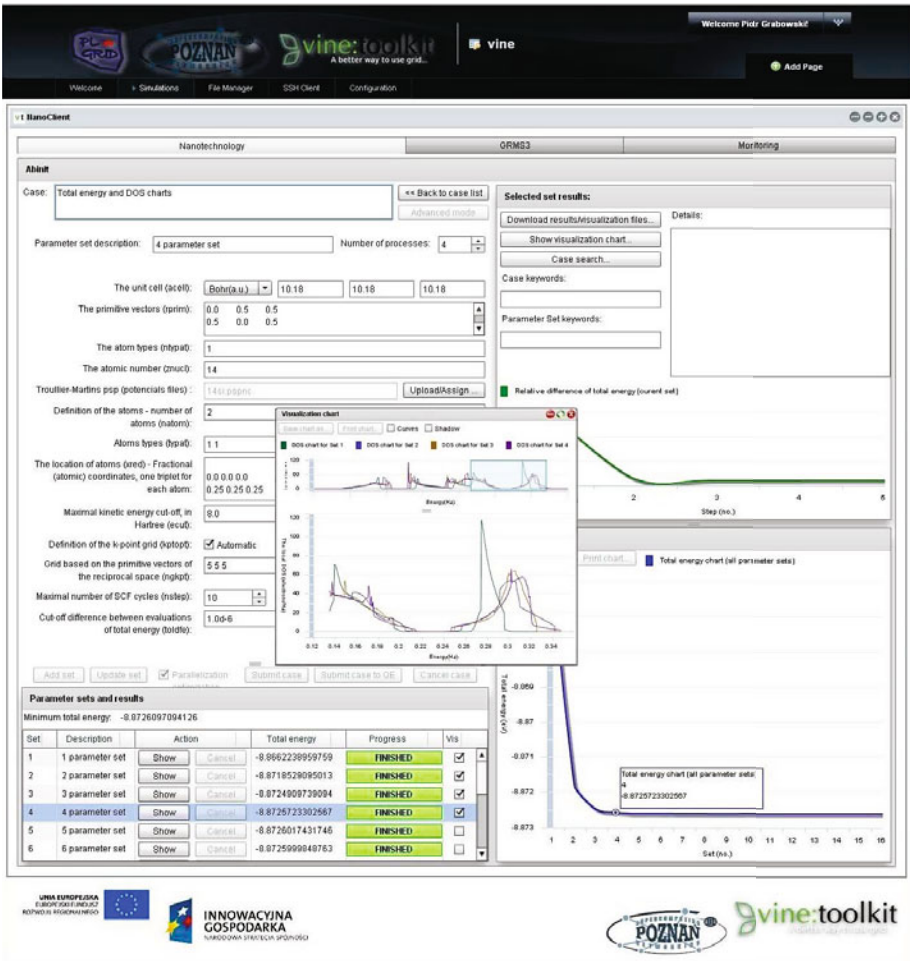

Fig. 1. Web-based interface for ABINIT simulation with DOS charts

Structure Builder does not cover all functionalities of the aforementioned applications; however, it enables ab inito creation of crystal structures, their edition and manipulation.

Nano Structure Builder has been divided into two separate web-based components: NanoBuilder and NanoEditor. The first generates geometry of crystallographic coordinates of at least one of the 230 symbols of symmetry group in the Hermann-Mauguin notation and lattice vectors and angles. The generated results are passed to NanoEditor. NanoEditor exploits the received coordinates of all atoms in the cell, in accordance with established symmetry, to generate graphical representation of the cell. The cell can be manually edited and modified with the provided tools. Moreover, the results obtained in that process can be saved as a file, and, thus, further used as an input to ABINIT.

NanoBuilder was created using the Adobe FLEX technology, wrapping the Spacegroup software. Spacegroup is a command line tool, which produces a crystal geometry; however, it can be used only under Unix systems. NanoBuilder gives its users an opportunity to use the tool within a web browser: defining basic information (space group by its Hermann-Mauguin symbol, lattice vectors lengths, lattice angles, number of unit cells in each direction and whether a unit cell should be found), adding atoms (by selecting them from a displayed periodic table) and defining position of each of the atoms. All these information is, invisibly to the user, passed to the Spacegroup software, which returns results as an output file.

NanoEditor is a graphical tool, which was also created in FLEX technology. It enables displaying a crystal cell in three dimensions. To achieve such a functionality, the Papervision3D library – an open source real-time 3D engine for the Flash platform – was used. The main purposes of using NanoEditor are: creation, edition and manipulation of super-cells. First, the user loads results obtained in NanoBuilder by selecting a proper file in a File Browser. When the file is loaded, its graphical representation is displayed in the middle panel of the component (Fig. 2). NanoEditor provides a whole set of tools to navigate and manipulate the model. The user can freely rotate it in any direction, or shift it, if the model does not fit entirely in the window. There is also a possibility to zoom in and zoom out the model, which is helpful when viewing the details of the cell. A very helpful feature of the tool is the ability to use two coordinate systems: Cartesian and cell coordinate system. Such distinction is needed because of the different functions available in the application. The first can be used when a new atom is added (coordinates need to be defined along x, y and z axis). The latter, in turn,

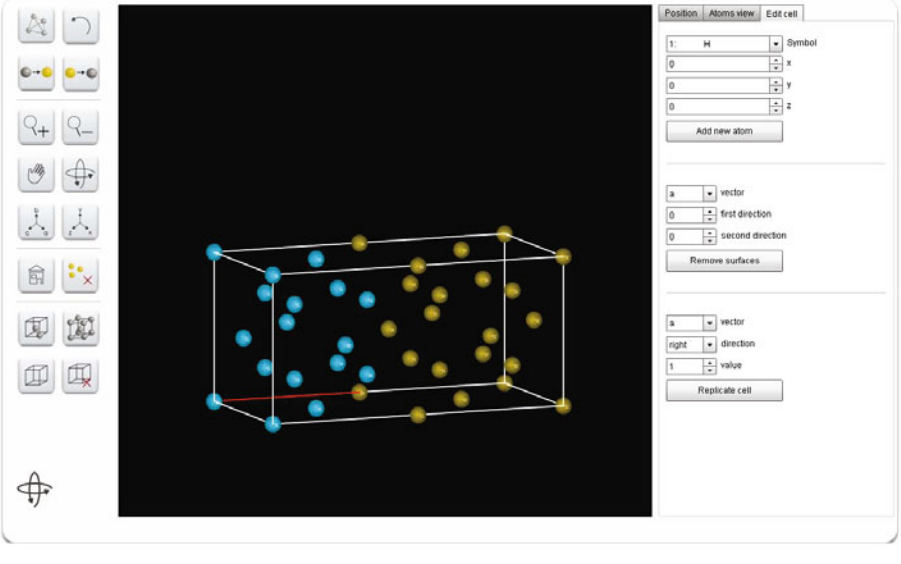

Fig. 2. Model of a unit cell displayed in a 3 dimensions

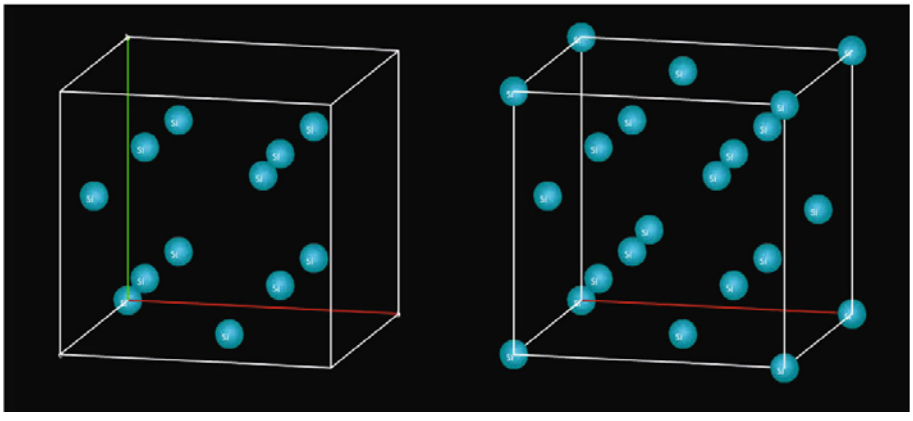

Fig. 3. Difference between primitive cell (on the left side) and the unit cell (on the right side)

helps to recognize directions of the cell when, for instance, some surface needs to be removed (surface is defined along a, b or c axis). The user can display any of the coordinate system or hide both of them.

There is also a possibility to show (and hide) the border of a crystal cell, which is helpful when identifying a crystal system. Moreover, the user is able to switch between two display modes of the unit cell. By design, a crystal cell is displayed as a primitive cell (translational asymmetric unit). But there is an additional option – displaying a nicely-cut unit cell (shortly unit cell). The difference between both cell views is demonstrated in Fig. 3. The unit cell displays additional atoms in places where multiplied cells are connected after the cell multiplication process.

A crucial functionality of NanoEditor is the edition of a crystal cell. The tool enables selection of a single atom or group of atoms, which can be further altered. It is possible to remove selected atoms and to change their positions by shifting them by, provided in Angstroms, values along each axis. To check the current position of an atom, the user can display it after selecting a proper atom. What is more, the user can display the distance between any pair of atoms. In addition, the user can add a new atom at every position. NanoEditor enables also replicating a whole cell a specified number of times along selected lattice vector. It can be done in both primitive and unit display modes. After achieving a desired form of a cell, the user can define vacuums. It is done by removing proper surfaces of the crystal cell. All the actions mentioned above, except for defining the vacuum, can be undone. It allows the users to make alterations without worrying about irreparable consequences. Such functionality was provided on account of the fact that users are prone to make some errors and like to have an ability to go back.

The last, but not least, important functionality of NanoEditor is its ability to display model parameters in ABINIT file format. Such parameters include: number of atoms, lattice vectors, cell angles, atom types and many more. After copying such output, the user can paste it as an input to another nano product

– Nano-Science Gateway. Thanks to that, the obtained model can be further processed and used.

The presented editor has become a really useful application for nano scientists who tested its prototype. They were able to design a nano structure without a need to have access to very extensive specialist software packages, like GoVasp. The source code is distributed as open source, therefore, it could be further developed in the future. It is also a great example of how we can use Vine mechanisms to prepare advanced graphical tools for end users.

In order to show how the described components are placed within a portal, we present the following diagram (Fig. 4). It depicts the elements of the portal, underlying services and dependencies between them.

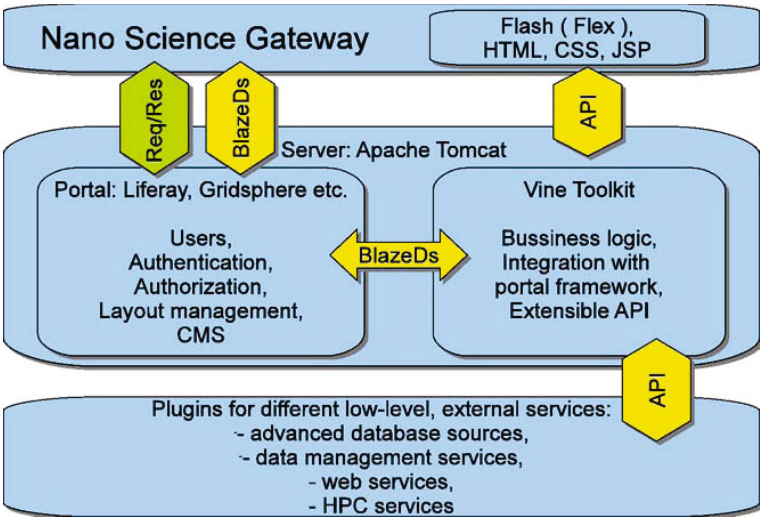

Fig. 4. Science Gateway deployment diagram

The Science Gateway for Nanotechnologists consists of two kinds of components available to a logged-in user: standard Vine Toolkit components for managing user profile, file management and SSH client; and specialized components designed for Nanotechnology environments. Both component groups are designed according to specific rules of grid portal design, based on the work conducted within the BEinGrid project [29]. One of the most important portal design rule is incorporating Single Sign-On mechanisms. In our Science Gateway it is fully supported, and based on Vine Toolkit – the user has to authenticate himself/herself only once, during the login procedure; then, all the credentials needed for accessing external services are automatically used by the portal on the user's account. It means, that even if the user needs to access a remote host with the Portal SSH Client (the researchers strongly indicated such a need in a survey conducted by the PL-Grid project), the process of authentication is performed entirely by the portal – the only thing the user has to do, is to choose appropriate resource. The same applies to the Science Gateway File Manager application

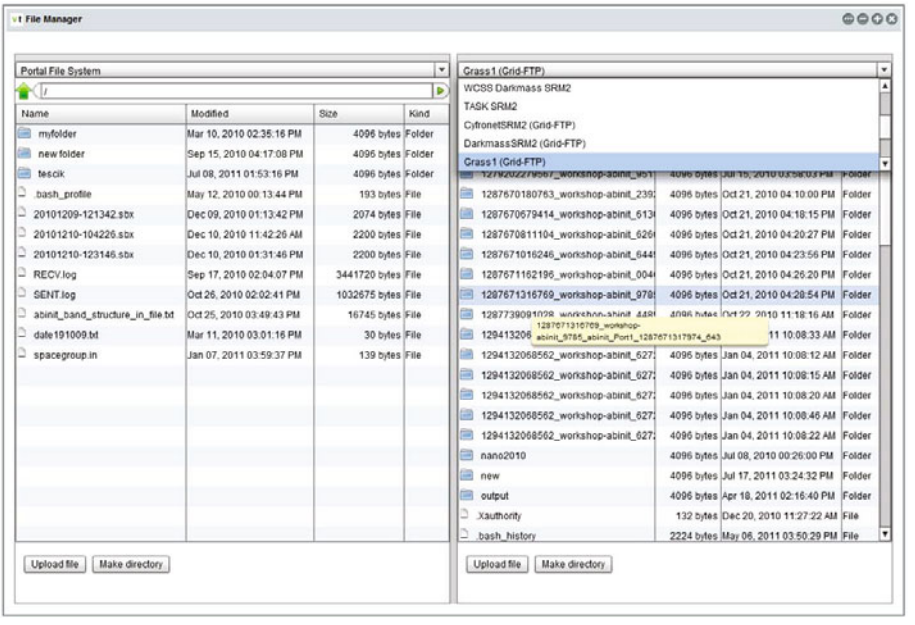

Fig. 5. Vine Toolkit File Manager with Single Sign-On

(Fig. 5). For ease-of-use, it consists of two panels (each for one storage resource). The user can make all standard file operations (e.g. copy files between panels with drag and drop interface, delete, create folders, change names, download or upload files) without the need to authenticate again.

5 Future Work

The future work on the Vine Toolkit-based Science Gateways are divided into two parts. The first are various new extensions to the existing Science Gateways, including support for other applications and packages, like NAMD and MOPAC. The second, based on the end-users needs collected within the PL-Grid project, is adding several new applications to the Science Gateways, e.g. NWChem or BLAST/CLUSTALW2. Therefore, our Science Gateways will be able to support all major applications used within large-scale parallel simulations in other science domains. In this way, rendering scientists able to deal with advanced calculations using web spaces that are easy to use and share.

References

1. Russell, M., Dziubecki, P., Grabowski, P., Krysiński, M., Kuczyński, T., Szjenfeld, D., Tarnawczyk, D., Wolniewicz, G., Nabrzyski, J.: The Vine Toolkit: A Java Framework for Developing Grid Applications. In: Wyrzykowski, R., Dongarra, J., Karczewski, K., Wasniewski, J. (eds.) PPAM 2007. LNCS, vol. 4967, pp. 331–340. Springer, Heidelberg (2008)

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 11(2), 161–172 (2011)
3. Dziubecki, P., Grabowski, P., Krysinski, M., Kuczynski, T., Kurowski, K., Szejnfeld, D.: Nano-Science Gateway development with Vine Toolkit and Adobe Flex. In: Barbera, R., Andronico, G., La Rocca, G. (eds.) Proceedings of the International Workshop on Science Gateways (IWSG 2010). Consorzio COMETA, Catania (2010)
4. 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 27(4), 357–369 (2011) ISSN 0167-739X, doi:10.1016/j.future.2010.11.015
5. Kurowski, K., de Back, W., Dubitzky, W., Gulyás, L., Kampis, G., Mamonski, M., Szemes, G., Swain, M.: Complex System Simulations with QosCosGrid. In: Allen, G., Nabrzyski, J., Seidel, E., van Albada, G.D., Dongarra, J., Sloot, P.M.A. (eds.) ICCS 2009, Part I. LNCS, vol. 5544, pp. 387–396. Springer, Heidelberg (2009), doi:10.1007/978-3-642-01970-8_38
6. Streit, A., Bala, P., Beck-Ratzka, A., Benedyczak, K., Bergmann, S., Breu, R., Daivandy, J. M., Demuth, B., Eifer, A., Giesler, A., Hagemeier, B., Holl, S., Huber, V., Lamla, N., Mallmann, D., Memon, A. S., Memon, M. S., Rambadt, M., Riedel, M., Romberg, M., Schuller, B., Schlauch, T., Schreiber, A., Soddemann, T., Ziegler, W.: UNICORE 6 – Recent and Future Advancements. JUEL-4319 (2010) ISSN 0944-2952
7. gLite 3, `http://glite.cern.ch/introduction`
8. GRIA 5.3, `http://www.gria.org/about-gria/overview`
9. Foster, I.: Globus Toolkit Version 4: Software for Service-Oriented Systems. In: Jin, H., Reed, D., Jiang, W. (eds.) NPC 2005. LNCS, vol. 3779, pp. 2–13. Springer, Heidelberg (2005)
10. Moor, R.: Towards a Theory of Digital Preservation. The International Journal of Digital Curation 3(1) (2008)
11. Rajasekar, A., Wan, M., Moore, R., Schroeder, W., Kremenek, G., Jagatheesan, A., Cowart, C., Zhu, B., Chen, S., Olschanowsky, R.: Storage Resource Broker – Managing Distributed Data in a Grid. Computer Society of India Journal, Special Issue on SAN 33(4), 42–54 (2003)
12. Antonioletti, M., Atkinson, M.P., Baxter, R., Borley, A., Chue Hong, N.P., Collins, B., Hardman, N., Hume, A., Knox, A., Jackson, M., Krause, A., Laws, S., Magowan, J., Paton, N.W., Pearson, D., Sugden, T., Watson, P., Westhead, M.: The Design and Implementation of Grid Database Services in OGSA-DAI. Concurrency and Computation: Practice and Experience 17(2-4), 357–376 (2005)
13. Foster, I., Grimshaw, A., Lane, P., Lee, W., Morgan, M., Newhouse, S., Pickles, S., Pulsipher, D., Smith, C., Theimer, M.: Open Grid Services Architecture Basic Execution Service Version 1.0 GFD-R.108 (2008), `http://www.ggf.org/documents/GFD.108.pdf`
14. Anjomshoaa, A., Brisard, F., Drescher, M., Fellows, D., Ly, A., McGough, S., Pulsipher, D., Savva, A.: Job Submission Description Language (JSDL) Specification, Version 1.0. GFD-R.056 (2005), `http://www.ggf.org/documents/GFD.56.pdf`
15. OGSA Resource Usage Service, `http://forge.ggf.org/sf/projects/rus-wg`

16. Microsoft's Active Directory, http://www.microsoft.com/windowsserver2008/en/us/active-directory.aspx
17. Oleksiak, A., Tullo, A., Graham, P., Kuczynski, T., Nabrzyski, J., Szejnfeld, D., Sloan, T.: HPC-Europa single point of access as a framework for building science gateways: Research Articles. Concurrency and Computation: Practice & Experience 19(6), 851–866 (2007)
18. P-GRADE, http://www.p-grade.hu/
19. EnginFrame, http://www.nice-software.com/web/nice/products/enginframe
20. SAGA, http://saga.cct.lsu.edu/
21. Klimeck, G., McLennan, M., Brophy, S.P., Adams III, G.B., Lundstrom, M.S.: nanoHUB.org: Advancing Education and Research in Nanotechnology. Computing in Science and Engineering 10(5), 17–23 (2008), doi:10.1109/MCSE.2008.120
22. myExperiment, http://www.myexperiment.org/
23. Guim, F., Rodero, I., Corbalan, J., Labarta, J., Oleksiak, A., Kuczynski, T., Szejnfeld, D., Nabrzyski, J.: Uniform job monitoring in the HPC-Europa project: data model, API and services. International Journal of Web and Grid Services 3(3), 333–353 (2007)
24. 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, P., 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, 2582–2615 (2009)
25. Gonze, X., Rignanese, G.-M., Verstraete, M., Beuken, J.-M., Pouillon, Y., Caracas, R., Jollet, F., Torrent, M., Zerah, G., Mikami, M., Ghosez, P., 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, 558–562 (2005)
26. Adobe, Flex/BlazeDs, http://www.adobe.com/products/flex/
27. Kokalj, A.: Computer graphics and graphical user interfaces as tools in simulations of matter at the atomic scale. Comp. Mat. Sci. 28, 155–168 (2003)
28. GoVASP, http://www.govasp.com/
29. Karanastasis, E., Varvarigou, T., Grabowski, P.: Portals for Service Oriented Infrastructures. In: Dimitrakos, T., Martrat, J., Wesner, S. (eds.) Service Oriented Infrastructures and Cloud Service Platforms for the Enterprise, pp. 159–177. Springer, Heidelberg (2010) ISBN 978-3-642-04085-6
30. Vine-users mailing list, http://gforge.man.poznan.pl/mailman/listinfo/vine-users
31. Kocot, J., Szepieniec, T., Noga, K., Harężlak, D., Sterzel, M.: InSilicoLab – Managing Complexity of Chemistry Computations. In: Bubak, M., Szepieniec, T., Wiatr, K. (eds.) PL-Grid 2011. LNCS, vol. 7136, pp. 265–275. Springer, Heidelberg (2012)
32. Ciepiela, E., Nowakowski, P., Kocot, J., Harężlak, D., Gubała, T., Meizner, J., Kasztelnik, M., Bartyński, T., Malawski, M., Bubak, M.: Managing Entire Lifecycles of e-Science Applications in the GridSpace2 Virtual Laboratory – from Motivation through Idea to Operable Web-Accessible Environment Built on Top of PL-Grid e-Infrastructure. In: Bubak, M., Szepieniec, T., Wiatr, K. (eds.) PL-Grid 2011. LNCS, vol. 7136, pp. 228–239. Springer, Heidelberg (2012)