



# Vine Toolkit

**vine:toolkit**  
open-source java grid application framework

## Distributed resources at your fingertips for developers and end users

### Main features:

- Single Sign-On – users log in once and use all resources
- Support for different grid infrastructures
- Advanced web applications (integration with Adobe Flex / BazeDS technology)
- Extensible, module based open architecture based on plugins
- Many applications included „out-of-the-box” such as: Job Manager, File Manager, Resource Manager, Credential Manager, Certificate Manager, GSI-SSHTerm applet
- Support for scientific applications: ABINIT, Quantum Espresso (and others...)
- Integration with portal environments Liferay and GridSphere installed on Tomcat server

### For whom:

- web applications developers** – a base for building advanced computational scientific portal gateways and applications with many ready to use components, integration layer for portal frameworks and advanced installation engine
- administrators of grid infrastructures** – possibility of deployment of a web portal “out-of-the-box” to access existing grid infrastructure
- end users** – many ready to use web applications for grid computations and data management in grid infrastructure
- scientists** – dedicated web applications for scientific applications for different scientific domains

### General description:

Vine Toolkit was designed as an environment to facilitate the development and integration of web-based applications with HPC resources, Grid services and various existing large-scale computing infrastructures managed by Grid middleware, such as gLite, Unicore, Globus, QosCosGrid and GRIA. It is possible to create a computational web-based Science Gateway using a modular structure and existing Vine components. Consequently, an easy-to-use presentation layer can be deployed together with various collaborative and visualization tools to simplify the way researchers, from different scientific domains, perform intensive computing studies and share data between simulations via lightweight web interfaces. Vine - together with a set of built-in modular components - is an excellent solution to establish web gateways for advanced scientific and engineering applications with grid-enabled resources in the backend. Moreover, the heterogeneity of Grid services and HPC resources can be unified thanks to Vine APIs and built-in capabilities for remote job submission, monitoring and control as well as data and workflow management, security and user management. Thus, integrating existing Vine modules and adding application-specific extensions it is possible to create a sophisticated Science Gateways to support collaborative scientific research.

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 support only 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. 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. Therefore, with a single software stack it is possible to build a complex solution consisting of the services, portal and set of user-customized applications at once available 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. Since version 1.1 Vine Toolkit supports also Liferay JSR-286 enterprise portal. 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.

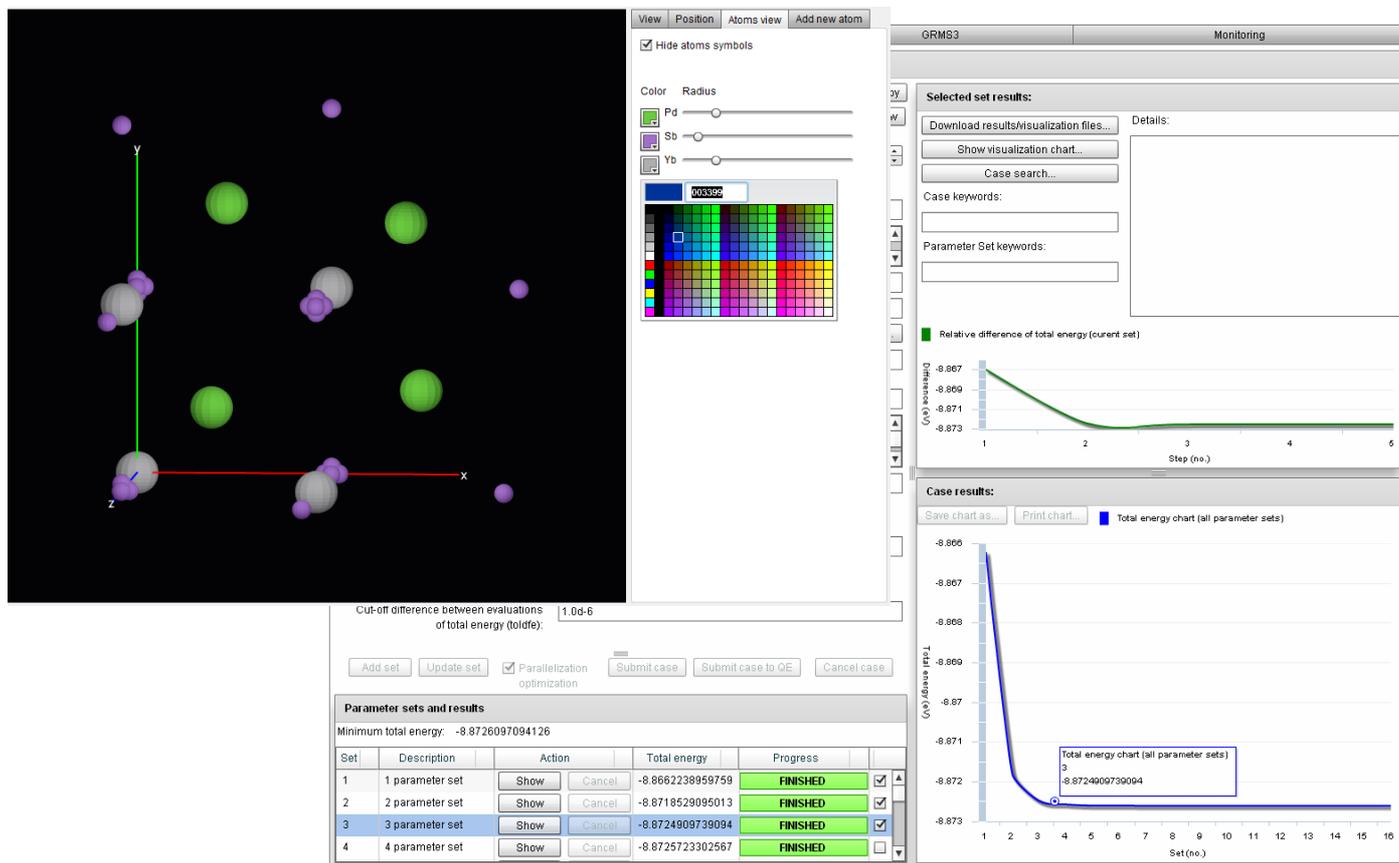




### Nano-technology portal gateway (<http://nano.man.poznan.pl>):

An example science gateway was recently developed and deployed under the PL-Grid infrastructure project. In fact, it was a joint research and development effort with researchers interested in collaborative, Web2.0 and large-scale simulation studies based on Density Functional Theory (DFT) and Many-Body Perturbation Theory. Thus, we selected a key software package called ABINIT and created from scratch many new and advanced web-based applications around it. In a nutshell, the ABINIT simulation software package allows 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 a planewave basis. 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 many capabilities, ABINIT provides only command-line tools. Moreover, it requires from its users not only domain-specific knowledge, but also a lot of expertise in computer science, and experiences with specific data formats and structures. 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 for 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. Moreover, Nano-Science Gateway was successfully presented at the NANO 2010 workshop attached to the 4th National Conference on Nanotechnology.



Example of the advanced web interface in the Nano-Science Gateway based on Vine Toolkit

Vine Toolkit has been and is developed within such projects like OMII-Europe, BEinGRID and PL-GRID.

