New Science Gateways for Advanced Computing Simulations and Visualization Using Vine Toolkit in PL-Grid

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PSNC
Agenda

- Vine Toolkit introduction
- Vine Toolkit – features
- Flex vs Silverlight
- Vine vs JSAGA
- Web portal with Vine Toolkit
- Bundled components
- OGF Standards (JSDL, BES)
- Flowify Portal
  - Nano-Science Gateway for PL-Grid project
- Next steps
Vine Toolkit introduction

- A modular and extensible Java/Flex based framework under Apache 2.0 license
- Derived from Grid Portlets for GridSphere
- Developed within EU funded projects: OMII-Europe, BEinGRID, HPC-Europa2
- Currently is being applied to the Polish NGI portal during the PL-Grid - Polish infrastructural project
- http://vinetoolkit.org/ - project web page, download, documentation, demos
Main target – **web applications** (could be a portlet, servlet, web service backend)

Integration with **different portal frameworks**, including well known web products like **GridSphere 3.1/3.2** and **Liferay 5.2.3**

**Ant based** installer; automatic, simple installation integrated with **svn**
- Installation support for **Tomcat 5/5.5/6.0**

Advanced **BlazeDs data services** improve the client-server communication to develop highly interactive and dynamic web applications
Vine Toolkit - features

- **Adobe Flex/Flash** technology allows creating advanced and sophisticated web interfaces similar to many stand-alone GUls.
- Other web GUI technologies could be supported (i.e. HTML, JavaScript with Ajax support).
- Uniform common API exposed to the end user which *abstracts* various middleware implementations.
- Extensible model for executing tasks (every action is persisted as *task*).
- Generic **resource based model** - any services and data sources can be integrated with web applications using high-level APIs.
## Abode Flex vs MS Silverlight

<table>
<thead>
<tr>
<th>Examined Feature</th>
<th>Adobe Flex</th>
<th>Microsoft Silverlight</th>
</tr>
</thead>
<tbody>
<tr>
<td>Charts support</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>CSS styles</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>Integration with JavaScript</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Printing</td>
<td>Yes</td>
<td>Not directly</td>
</tr>
<tr>
<td>SDK availability</td>
<td>Yes, all platforms, open source (Flex SDK). Flash Builder (Windows, Mac Os), paid.</td>
<td>Yes, Windows (.NET), paid, Unix (Mono not compatible with the latest Silverlight)</td>
</tr>
<tr>
<td>Licence</td>
<td>Adobe Flex SDK: open-source (Mozilla Public License) BlazeDS: open-source (LGPL v3)</td>
<td>Proprietary MS-EULA</td>
</tr>
<tr>
<td>Languages</td>
<td>ActionScript, Mxml</td>
<td>C#, Visual Basic, XAML</td>
</tr>
<tr>
<td>Multi-threading</td>
<td>No</td>
<td>Yes (SL4)</td>
</tr>
<tr>
<td>Data Services</td>
<td>Yes (LifeCycle, BlazeDs)</td>
<td>Yes</td>
</tr>
<tr>
<td>Middleware</td>
<td>Vine toolkit</td>
<td>Saga – Java adaptors</td>
</tr>
<tr>
<td>----------------------------------</td>
<td>--------------</td>
<td>---------------------------------------</td>
</tr>
<tr>
<td>gLite 3 - Cream</td>
<td>Yes</td>
<td>Yes - JSAGA</td>
</tr>
<tr>
<td>gLite 3 - WMS</td>
<td>Yes</td>
<td>Yes - JSAGA</td>
</tr>
<tr>
<td>gLite 3 - JDL</td>
<td>Yes</td>
<td>under development - JSAGA</td>
</tr>
<tr>
<td>Globus Toolkit</td>
<td>Yes (4.0.x, 4.2.1)</td>
<td>Yes (up to 4.2) - JSAGA/JavaGAT</td>
</tr>
<tr>
<td>Globus Toolkit – MyProxy</td>
<td>Yes</td>
<td>Yes - JSAGA</td>
</tr>
<tr>
<td>Globus Toolkit – gsiftp</td>
<td>Yes</td>
<td>Yes - JSAGA</td>
</tr>
<tr>
<td>Globus Toolkit - WS-GRAM</td>
<td>Yes</td>
<td>Yes - JSAGA</td>
</tr>
<tr>
<td>BES</td>
<td>Yes</td>
<td>Yes - JSAGA</td>
</tr>
<tr>
<td>JSDL</td>
<td>Yes</td>
<td>Yes - JSAGA</td>
</tr>
<tr>
<td>GRIA</td>
<td>Yes (5.3)</td>
<td>No</td>
</tr>
<tr>
<td>Unicore 6</td>
<td>Yes</td>
<td>Yes - JSAGA</td>
</tr>
<tr>
<td>Active Directory</td>
<td>Yes</td>
<td>Yes - JSAGA</td>
</tr>
<tr>
<td>Java Keystore</td>
<td>Yes</td>
<td>Yes - JSAGA</td>
</tr>
<tr>
<td>X509 Certificates</td>
<td>Yes</td>
<td>Yes - JSAGA</td>
</tr>
<tr>
<td>Storage Resource Manager</td>
<td>Yes</td>
<td>Yes - JSAGA</td>
</tr>
<tr>
<td>Storage Resource Broker</td>
<td>Yes</td>
<td>Yes - JSAGA</td>
</tr>
<tr>
<td>(S)FTP, SSH, HTTP(S), ZIP</td>
<td>Partly (http, SSH applet)</td>
<td>Yes - JSAGA/JavaGAT</td>
</tr>
<tr>
<td>local data management</td>
<td>Yes</td>
<td>Yes - JSAGA</td>
</tr>
<tr>
<td>WebDav</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td>VOMS</td>
<td>Yes</td>
<td>Yes - JSAGA</td>
</tr>
<tr>
<td>iRODS</td>
<td>Work pending…</td>
<td>Yes - JSAGA</td>
</tr>
<tr>
<td>NAREGI (Super Scheduler)</td>
<td>No</td>
<td>Yes - JSAGA</td>
</tr>
<tr>
<td>QosCosGrid</td>
<td>Yes</td>
<td>No</td>
</tr>
</tbody>
</table>
Web portal with Vine Toolkit

GUI (layout + portlets)

- Req/Res
- BlazeDs

Portal: Liferay, Gridsphere etc.

- Users,
- Authentication,
- Authorization,
- Layout management,
- CMS

Server: Apache Tomcat

- Flash (Flex),
- HTML, CSS, JSP

Vine Toolkit

- Bussiness logic,
- Integration with portal framework,
- Extensible API

BlazeDs

API

Plugins for different low-level, external services:

- advanced database sources,
- data management services,
- web services,
- HPC services
Bundled components

- User / Roles / Application / Properties Manager - administrative tools

- Login / Registration components plugin based with a support for i.e. Active Directory, MyProxy, VOMS etc.

- Resource manager – configuration tool for the domain registry

- File browser component (support for the internal Portal File System and various file system protocols like GridFTP, LFC, SRM, Unicore SMS, iRODS)
Bundled components

- Job manager (submission, monitoring) generic component (based on JSDL) – support for Globus GT4, Unicore 6, gLite 3, QocCosGrid, GRIA
- Credential manager (including MyProxy support)
- Resource browser – information services client for MDS in GT4
- GSI-SSHTerm applet – SSH console available in the portal
- Kepler workflow editor (optional)
- Set of example components demonstrating Vine's UI features
OGF standards

- **JSDL v1.0** support
  - Application extensions:
    - **POSIXApplication** (default JSDL extension)
    - **HPCProfileApplication** (used with BES services)
    - **SPMDApplication** (translated with XSLT to define mpi jobs in GT4)

- **BES v1.0** (Basic Execution Service)
  - developed during OMII-Europe project and reimplemented later to support full HPCProfileApplication JSDL extension
  - tested with many BES compliant services like Unicore BES, CREAM-BES Computing Element, GT4 BES service, Chinese CROWN BES metascheduler service

- Vine Plugins use XSLT translation if JSDL is not supported (Glite WMS, Globus GT4, proprietary CE resource)
Flowify Portal

**Wow2green Portal**
- Manages users and roles
  - Administrator
- Creates and uploads a workflow
  - Workflow designer

**Vine Web Service**
- Kepler Web Service
  - Vine actors
  - GRMS broker
  - GRIA JSBSim Gnuplot
  - GRIA JSBSim Gnuplot
  - GRIA JSBSim Gnuplot

**Examples of some final result**

**Engineer**
- Creates a simulation
- Browses an output
- Uploads input data
- XML description of an experiment

**Team manager**
- Browses shared team simulations
Nano-Science Gateway for PL-Grid

- Large-scale simulation studies based on **Density Functional Theory (DFT)** and **Many-Body Perturbation Theory**
- Command line applications fired through **CosQosGrid** middleware as MPI application in batch mode
- **ABINIT** and **Quantum Espresso** both allows:
  - finding the total energy
  - finding charge density and electronic structure of systems made of electrons and nuclei within Density Functional Theory (DFT), using pseudopotentials and a planewave basis
  - optimize the geometry, perform molecular dynamics simulations, generate dynamical matrices, Born effective charges, and dielectric tensors according to the DFT forces and stresses
- 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**

**Simple and advanced mode** (user manually edits ABINIT input file)

**Dynamic charts** during computations and after completion (convergence of the relative difference between subsequent computation iterations, density of electronic states - DOS)

**Successfully presented** at the **NANO 2010 workshop** attached to the 4th National Conference on Nanotechnology
Nano-Science Gateway for PL-Grid

NanoToolkit

NanoToolkit is an example of science gateway that has been 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, a key software package called ABINIT was selected and many new and advanced web-based applications were created from scratch around it. Below are presented three of them, that enable edition and manipulation of crystal structures and large-scale simulation studies based on Density Functional Theory.

NanoBuilder - interface that allows to enter input data and generate 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. Generated coordinates of all atoms in the cell in accordance with established symmetry can then be used to render the cell, which may be subjected to a process of further processing in the NanoEditor.

NanoEditor - graphical tool that enables creating, processing super-cells and generating output files that can be further used in the Abinit package. By processing we mean cell replication operations, changing positions of certain atoms or groups of atoms within the cell, the addition of atoms and defining the vacuum.

NanoSimulator - it is an example of science gateway that has been 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, a key software package called ABINIT was selected and many new and advanced web-based applications were created from scratch around it.
Nano-Science Gateway for PL-Grid
Nano-Science Gateway for PL-Grid

Parameter set description:
- 1 parameter set
- Number of processes: 4
- The unit cell (a, b, c): 15.18, 15.18, 15.18
- The primitive vectors (a, b, c): 0.0, 0.5, 0.5
- 0.5, 0.0, 0.5
- The atom types (m, p, u): 1
- The atomic number (Z): 143246
- Troullier-Martins pop (potentials file): 1432_wc_hf_3pg_lcao_46-Pd_GGA_hf
- Definition of the atoms - number of atoms: 2
- Atomic types (m, p, u): 1
- The location of atoms (m, p, u): Fractional (atomic) coordinates, one triplet for each atom: 0.0, 0.0, 0.0, 0.25, 0.25, 0.25
- Maximal kinetic energy cut-off: 8.0 (Ha)
- Definition of the k-point grid (kopt): Automatic
- Grid based on the primitive vectors of the reciprocal space (kopt): 2X2X2
- Maximal number of SCF cycles (kopt): 10

Parameter sets and results

<table>
<thead>
<tr>
<th>Set</th>
<th>Description</th>
<th>Action</th>
<th>Total energy</th>
<th>Progress</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1 parameter set</td>
<td>Show</td>
<td>-7.8683239178963</td>
<td>FINISHED</td>
</tr>
<tr>
<td>2</td>
<td>1 parameter set</td>
<td>Show</td>
<td>-7.8683239178963</td>
<td>FINISHED</td>
</tr>
<tr>
<td>3</td>
<td>1 parameter set</td>
<td>Show</td>
<td>-7.8683239178963</td>
<td>FINISHED</td>
</tr>
</tbody>
</table>
Nano-Science Gateway for PL-Grid
Nano-Science Gateway for PL-Grid

The above image shows a graphical user interface for a molecular modeling tool. The interface includes a periodic table, a 3D molecular model editor, and various tools for manipulating the molecular structure. The tool allows for the creation, modification, and visualization of molecular structures.
Next steps

◆ PL-Grid project
  ♦ Liferay portal – software audit and later production deployment
    • Science Gateways integrated with ARU – central user management service
  ♦ More science gateways planned in domains like biotechnology, chemistry and others
◆ Nano-Science Gateway
  ♦ Extensions for Abinit and Quantum Espresso web applications
  ♦ Support for more nano applications planned
◆ HPC-Europa2 project
  ♦ Further development of data management web application for iRODS
Any questions, comments or remarks are very welcome.
contact: deepres@man.poznan.pl

Vine Toolikt: http://vinetoolkit.org/
Vine users mailing list: vine-users@gforge.man.poznan.pl
Nano-Science Gateway: http://nano.man.poznan.pl
QosCosGrid: http://larix.man.poznan.pl/wiki/QosCosGrid_Tutorial
http://node2.qoscosgrid.man.poznan.pl/gridsphere/gridsphere