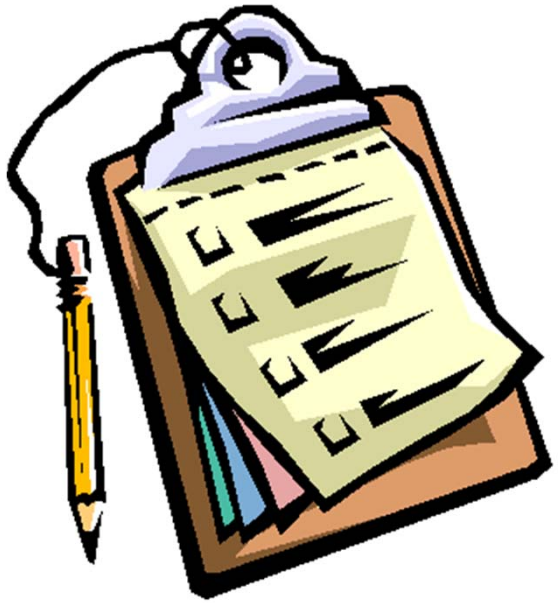
POZNAŃ SUPERCOMPUTING AND NETWORKING CENTER

Molecular Dynamics Science Gateway with Vine Toolkit providing Unicore middleware support

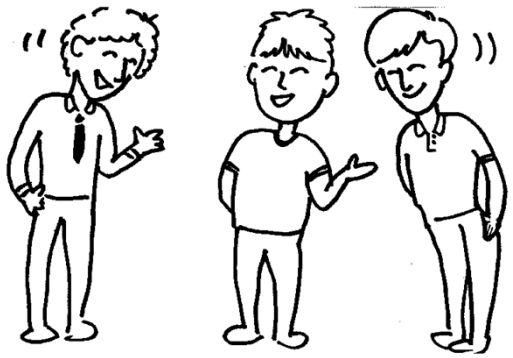
Piotr Dziubecki, Piotr Grabowski, Tomasz Kuczyński, Krzysztof Kurowski, Dawid Szejnfeld, Dominik Tarnawczyk, Małgorzata Wolniewicz
PSNC

Agenda



- Vine Toolkit introduction
- Vine Toolkit – features
- Web portal with Vine Toolkit
- Bundled components
- UNICORE 6 plugin
- OGF Standards (JSDL, BES)
- Molecular Dynamics Science Gateway
- Application registry
- Software stack and technologies
- User interface features
- Nano-Science Gateway
- Towards modern web applications (Facebook, iGoogle)
- Future plans

Vine Toolkit introduction



- A **modular and extensible** Java/Flex based framework
- 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

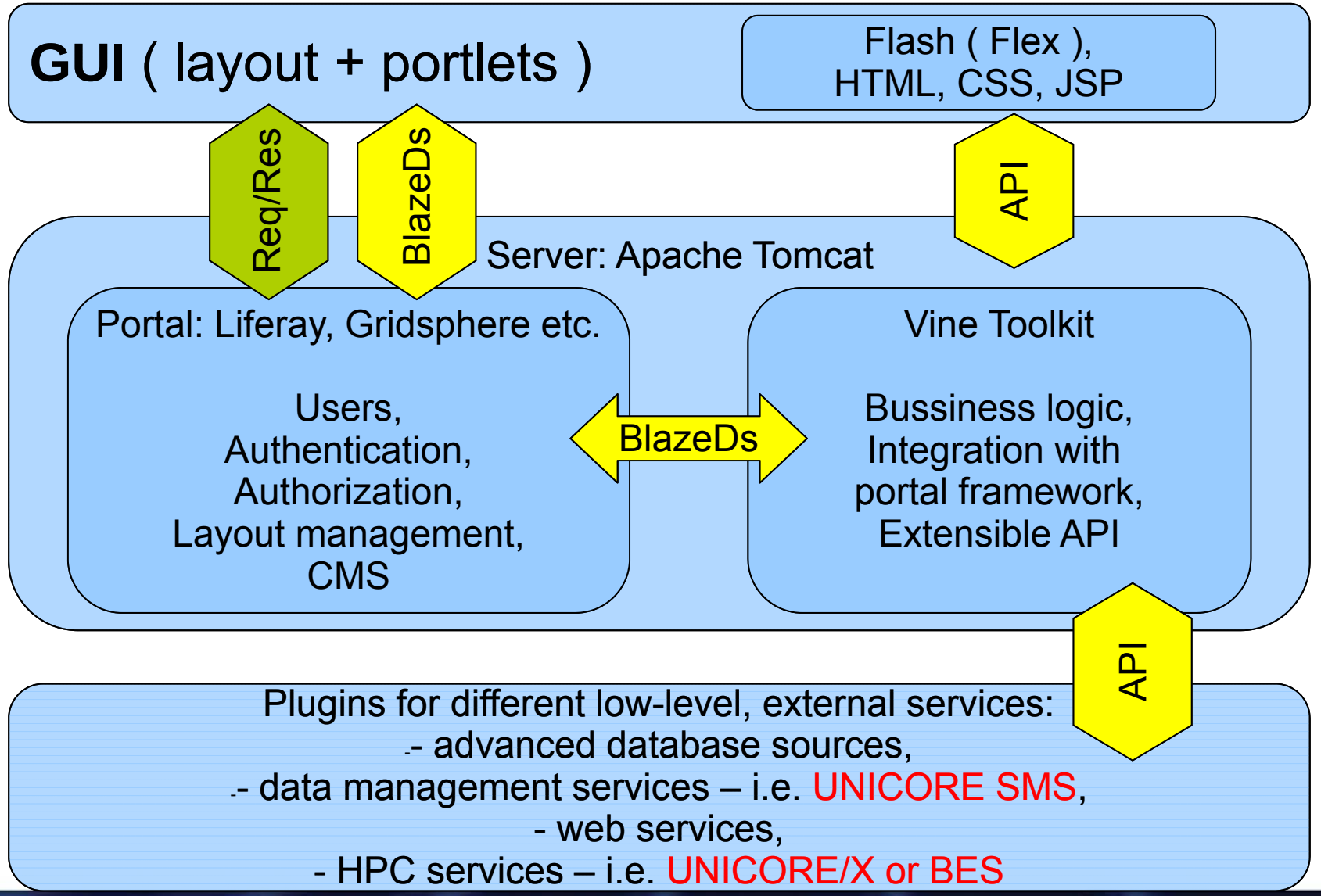
Vine Toolkit - features

- Integration with **different portal frameworks,** including well known web products like **GridSphere** and **Liferay**
- **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

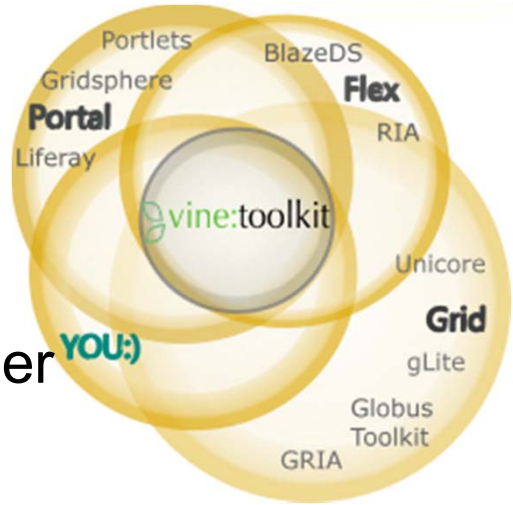
Vine Toolkit - features

- **Adobe Flex/Flash** technology allows creating advanced and sophisticated web interfaces similar to many stand-alone GUIs
- 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

Web portal with Vine Toolkit

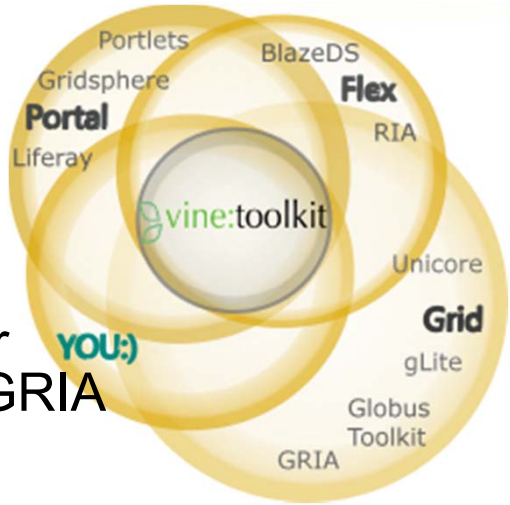


Bundled components



- User / Roles / Application / Properties Manager - administrative tools
- Login / Registration components plugin based with a support for i.e. Active Directory, MyProxy 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 **UNICORE 6**, Globus GT4, gLite 3, QocCosGrid, GRIA
- Credential manager (including MyProxy support) – proxy certificates used in portal
- Resource browser – information services client for MDS in GT4
- GSI-SSHTerm applet – SSH console available in the portal
- Set of example components demonstrating Vine's UI features

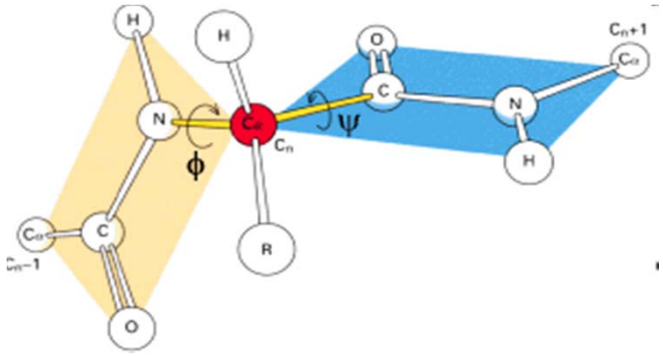
UNICORE 6 plugin

- Proxy certificates used so proxy certificate UNICORE Gateway extension is required – other middlewares also use them
- It is possible to configure also common portal certificate instead
- SAML Assertions could be possibly used in future – Java Web Start or Java Applet to generate user SAML Assertion (lifetime? How often user shoud create it and upload? It is passed to portal – weak point?)
- Plugin uses UCC jars – UNICORE/X and BES access possible
- Some fixes related to inner use of Ehcache, some classes overloaded, there were some multiuser access problems

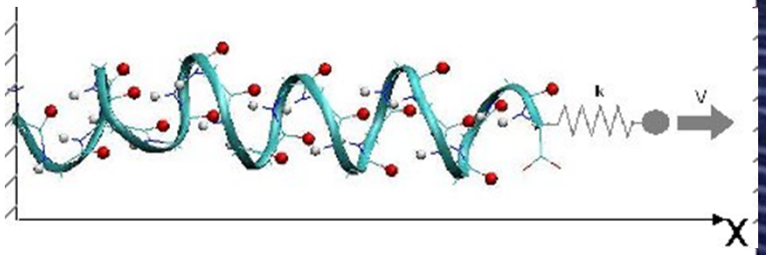
OGF standards

- **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)

Molecular Dynamics Science Gateway

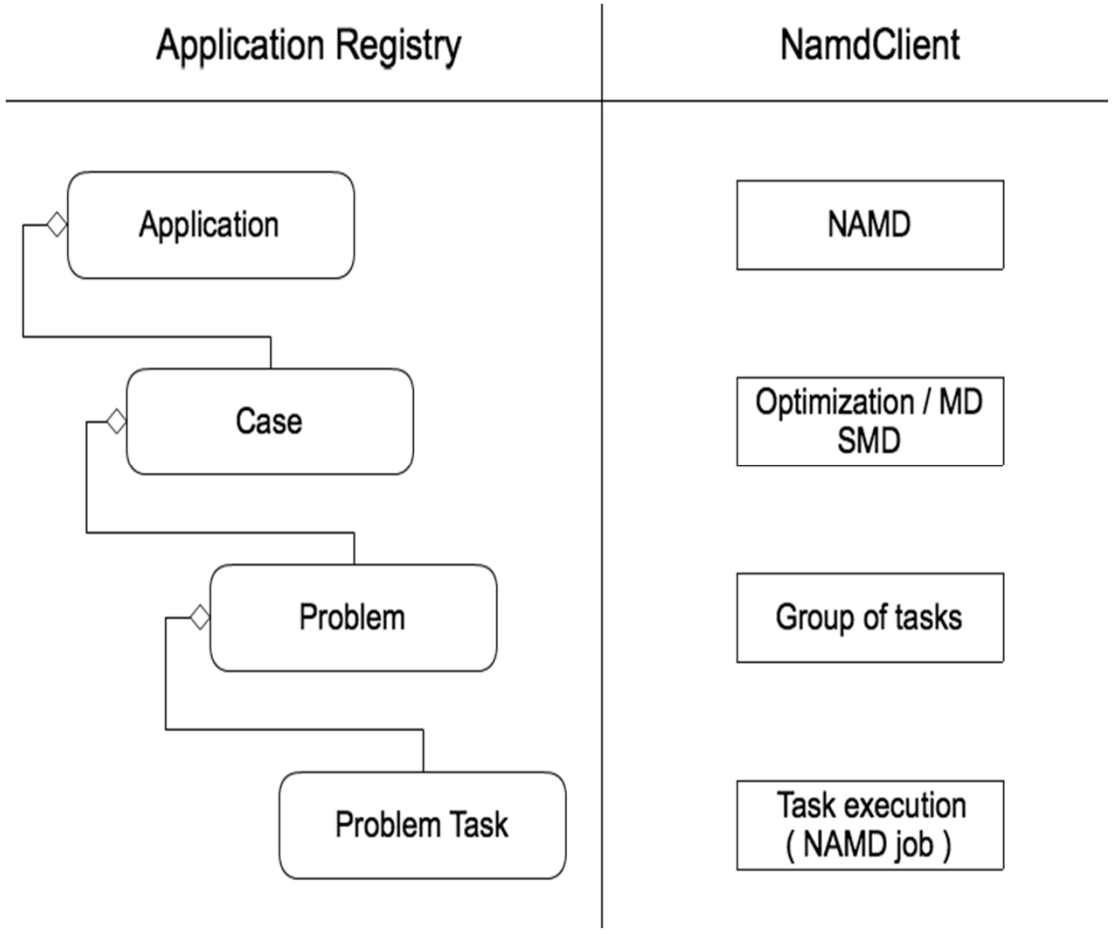


- The whole system is meant to solve molecular dynamics (MD) simulation problems
- Offers a profiled web interface to the NAMD application
- User uses external tool to build molecules like peptides for example (to create pdb, psf input files)
- Ability to load ready to use models from external databases like Protein Data Bank
- Input files like psf should be editable directly in the portal
- Number of parameters to set before simulation
- NAMD application exposed for end users on grid infrastructure
- Parallel optimilization (in general limited) vs multiple instance of problems (currently desired by end users)
- Goal: system geometry optimization (or) and simulation by molecular dynamics method (hours to days)
- Outputs: charts from generated log files: total energy (ETOTAL), kinetic energy (EKINETIC), bond, angle, ELEC, VDW etc.
- Still at early stage…but already tested with UNICORE



Application registry

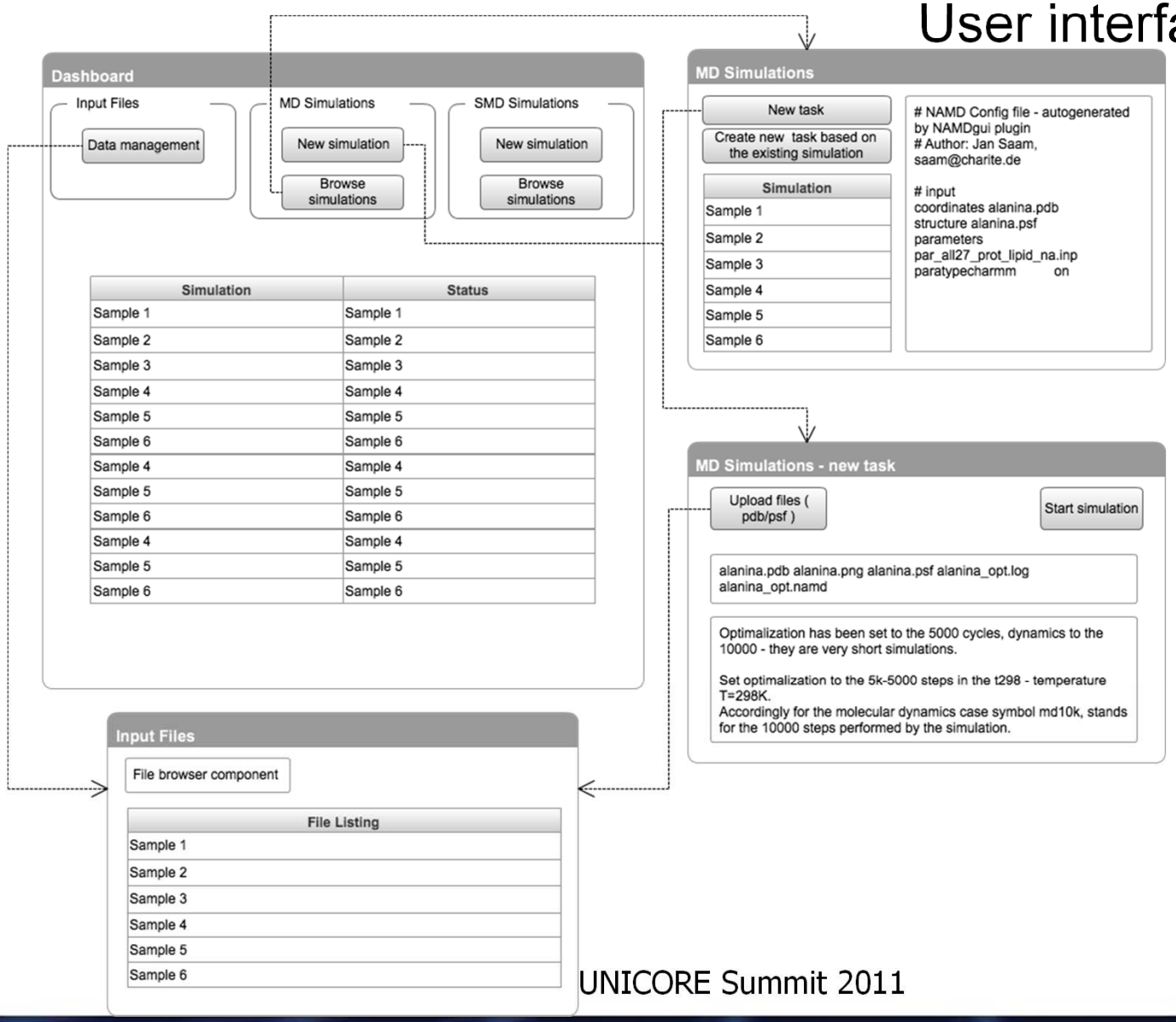
- Vine Application Registry and UI component
- scientific applications and simulations are mapped to logical entities
- full history of simulation runs with parameters and job descriptions – problem library
- log scrapping mechanism, which let us visualize the partial result in the realtime



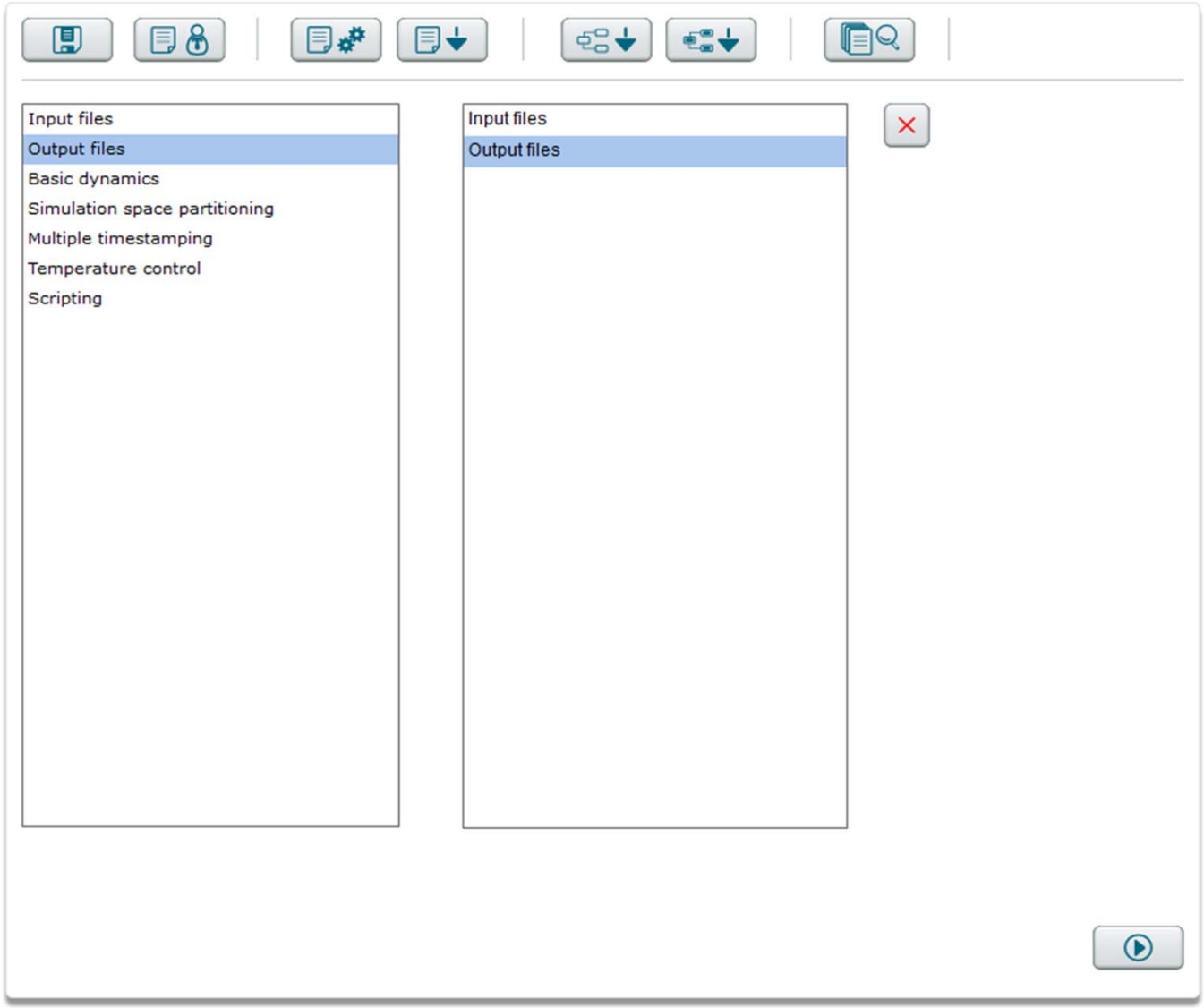
Software stack and technologies

Software stack	Technologies
NAMD Web Client	Adobe Flex / BlazeDS
Portal	Java / Portlets
Vine Toolkit framework	Java / Web Services
UNICORE middleware / other HPC resources and data services	Web Services / product specific implementations

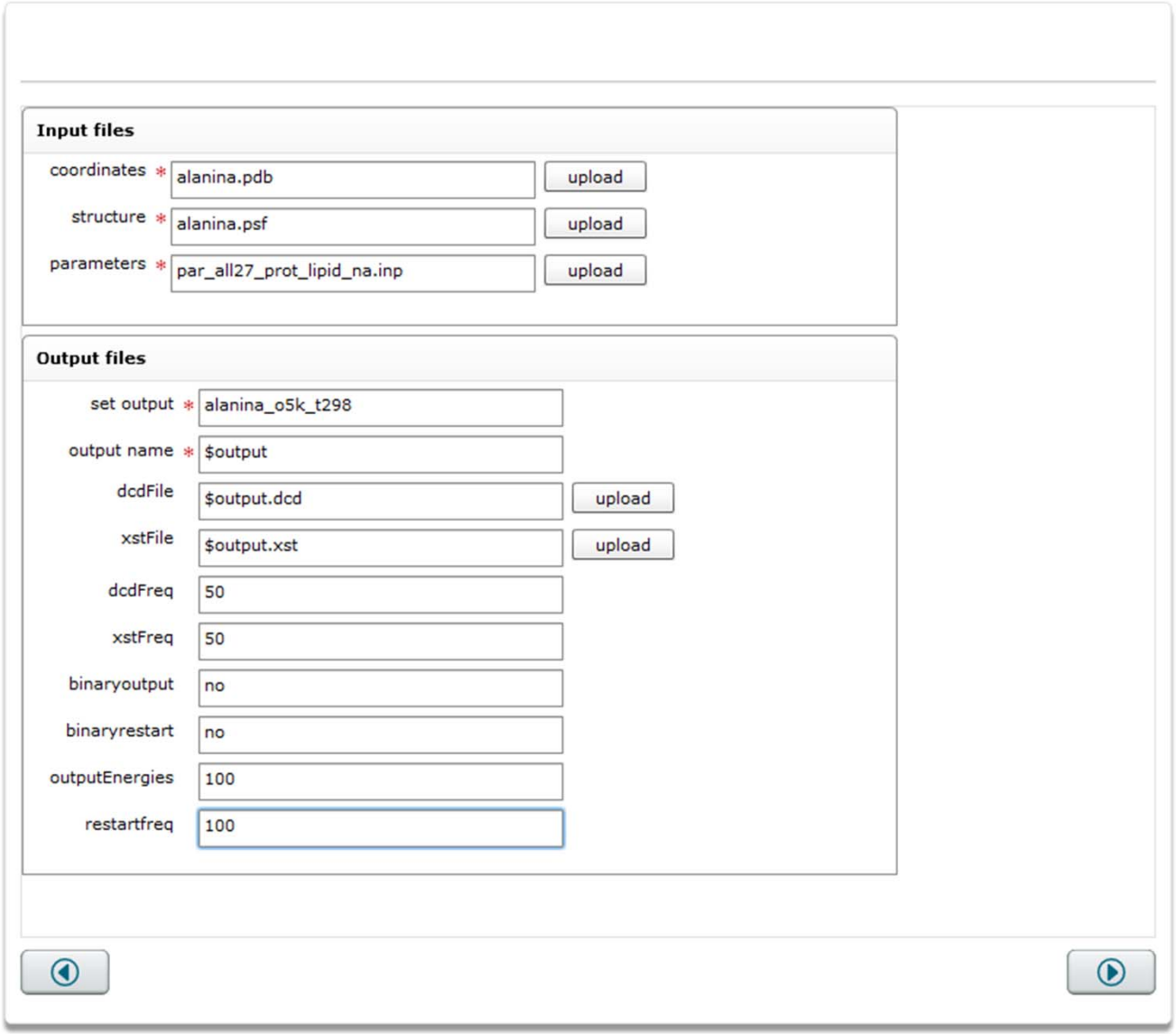
User interface features



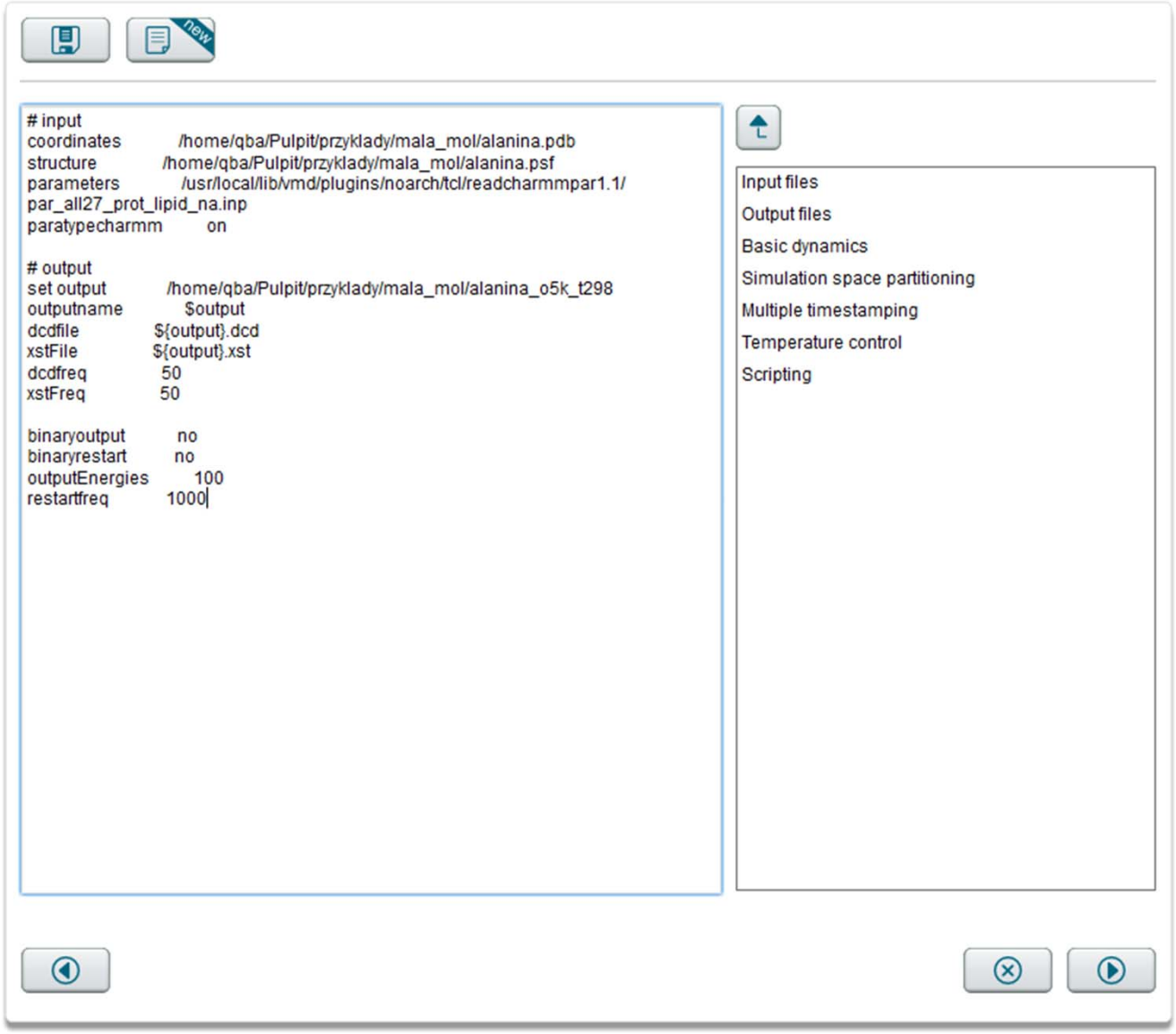
NAMD Client screenshots - .namd file configuration



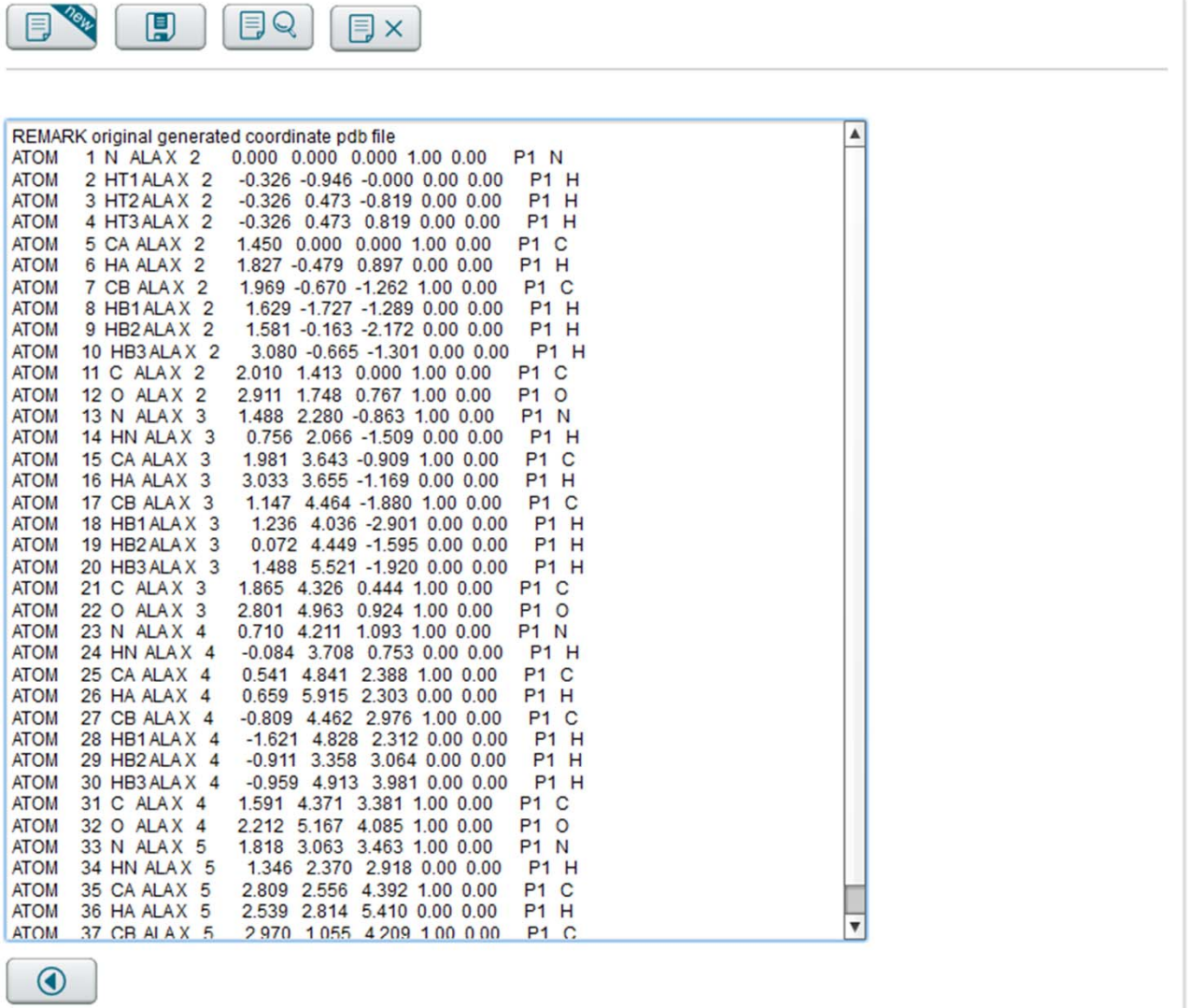
NAMD Client screenshots – further configuration



NAMD Client screenshots – .namd file ready to use



NAMD Client screenshots – pdb input file

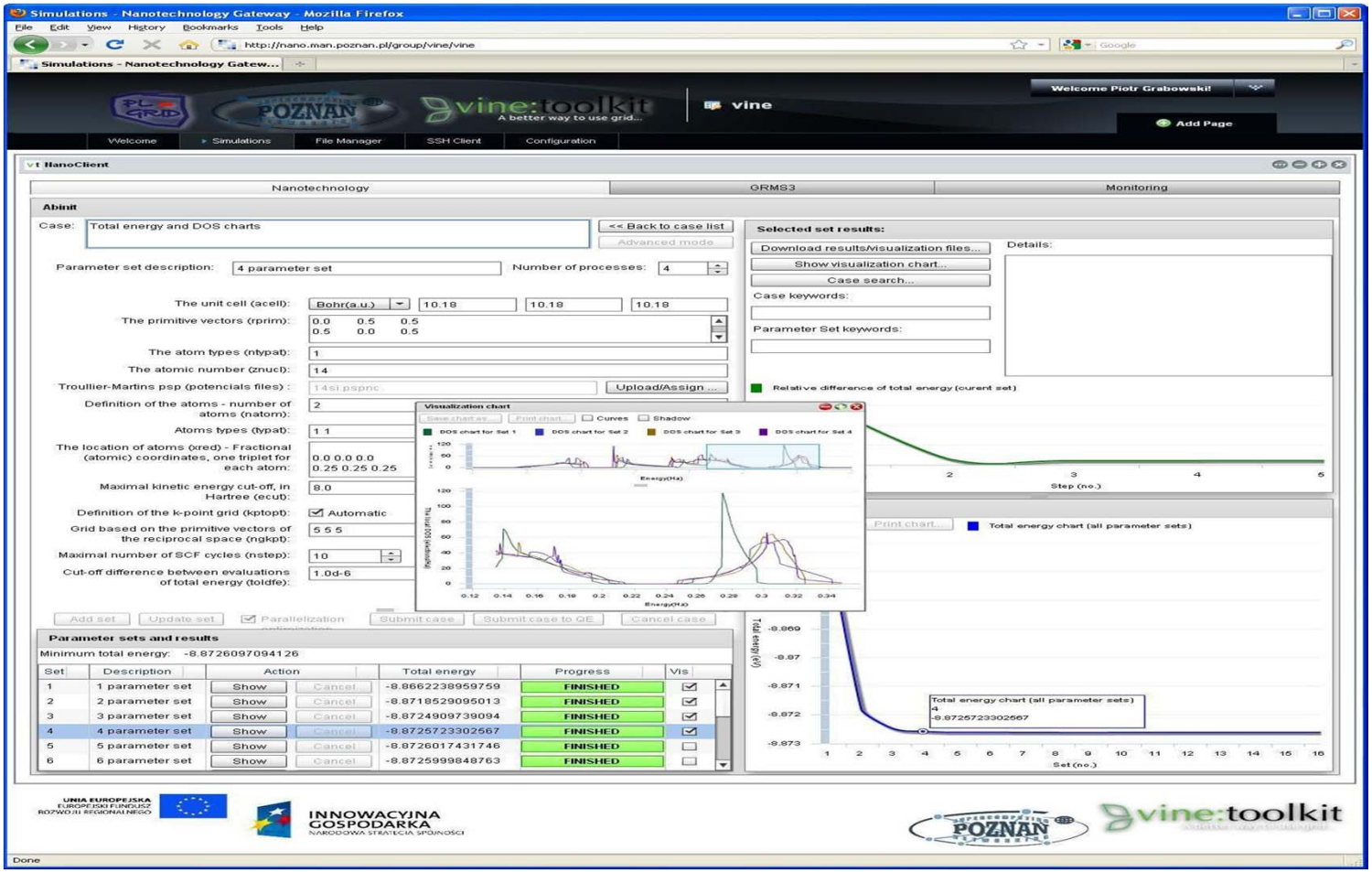


```
REMARK original generated coordinate pdb file
ATOM      1  N   ALA X   2       0.000   0.000   0.000  1.00  0.00      P1   N
ATOM      2  HT1 ALA X   2      -0.326  -0.946  -0.000  0.00  0.00      P1   H
ATOM      3  HT2 ALA X   2      -0.326   0.473  -0.819  0.00  0.00      P1   H
ATOM      4  HT3 ALA X   2      -0.326   0.473   0.819  0.00  0.00      P1   H
ATOM      5  CA  ALA X   2       1.450   0.000   0.000  1.00  0.00      P1   C
ATOM      6  HA  ALA X   2       1.827  -0.479   0.897  0.00  0.00      P1   H
ATOM      7  CB  ALA X   2       1.969  -0.670  -1.262  1.00  0.00      P1   C
ATOM      8  HB1 ALA X   2       1.629  -1.727  -1.289  0.00  0.00      P1   H
ATOM      9  HB2 ALA X   2       1.581  -0.163  -2.172  0.00  0.00      P1   H
ATOM     10  HB3 ALA X   2       3.080  -0.665  -1.301  0.00  0.00      P1   H
ATOM     11  C   ALA X   2       2.010   1.413   0.000  1.00  0.00      P1   C
ATOM     12  O   ALA X   2       2.911   1.748   0.767  1.00  0.00      P1   O
ATOM     13  N   ALA X   3       1.488   2.280  -0.863  1.00  0.00      P1   N
ATOM     14  HN  ALA X   3       0.756   2.066  -1.509  0.00  0.00      P1   H
ATOM     15  CA  ALA X   3       1.981   3.643  -0.909  1.00  0.00      P1   C
ATOM     16  HA  ALA X   3       3.033   3.655  -1.169  0.00  0.00      P1   H
ATOM     17  CB  ALA X   3       1.147   4.464  -1.880  1.00  0.00      P1   C
ATOM     18  HB1 ALA X   3       1.236   4.036  -2.901  0.00  0.00      P1   H
ATOM     19  HB2 ALA X   3       0.072   4.449  -1.595  0.00  0.00      P1   H
ATOM     20  HB3 ALA X   3       1.488   5.521  -1.920  0.00  0.00      P1   H
ATOM     21  C   ALA X   3       1.865   4.326   0.444  1.00  0.00      P1   C
ATOM     22  O   ALA X   3       2.801   4.963   0.924  1.00  0.00      P1   O
ATOM     23  N   ALA X   4       0.710   4.211   1.093  1.00  0.00      P1   N
ATOM     24  HN  ALA X   4      -0.084   3.708   0.753  0.00  0.00      P1   H
ATOM     25  CA  ALA X   4       0.541   4.841   2.388  1.00  0.00      P1   C
ATOM     26  HA  ALA X   4       0.659   5.915   2.303  0.00  0.00      P1   H
ATOM     27  CB  ALA X   4      -0.809   4.462   2.976  1.00  0.00      P1   C
ATOM     28  HB1 ALA X   4      -1.621   4.828   2.312  0.00  0.00      P1   H
ATOM     29  HB2 ALA X   4      -0.911   3.358   3.064  0.00  0.00      P1   H
ATOM     30  HB3 ALA X   4      -0.959   4.913   3.981  0.00  0.00      P1   H
ATOM     31  C   ALA X   4       1.591   4.371   3.381  1.00  0.00      P1   C
ATOM     32  O   ALA X   4       2.212   5.167   4.085  1.00  0.00      P1   O
ATOM     33  N   ALA X   5       1.818   3.063   3.463  1.00  0.00      P1   N
ATOM     34  HN  ALA X   5       1.346   2.370   2.918  0.00  0.00      P1   H
ATOM     35  CA  ALA X   5       2.809   2.556   4.392  1.00  0.00      P1   C
ATOM     36  HA  ALA X   5       2.539   2.814   5.410  0.00  0.00      P1   H
ATOM     37  CB  ALA X   5       2.970   1.055   4.209  1.00  0.00      P1   C
```

Nano-Science Gateway

- Large-scale simulation studies based on **Density Functional Theory (DFT)** and **Many-Body Perturbation Theory**
- Command line applications fired through **CosQosGrid** middleware (other could be used like UNICORE 6) 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, **another workshop just took place in July 2011**

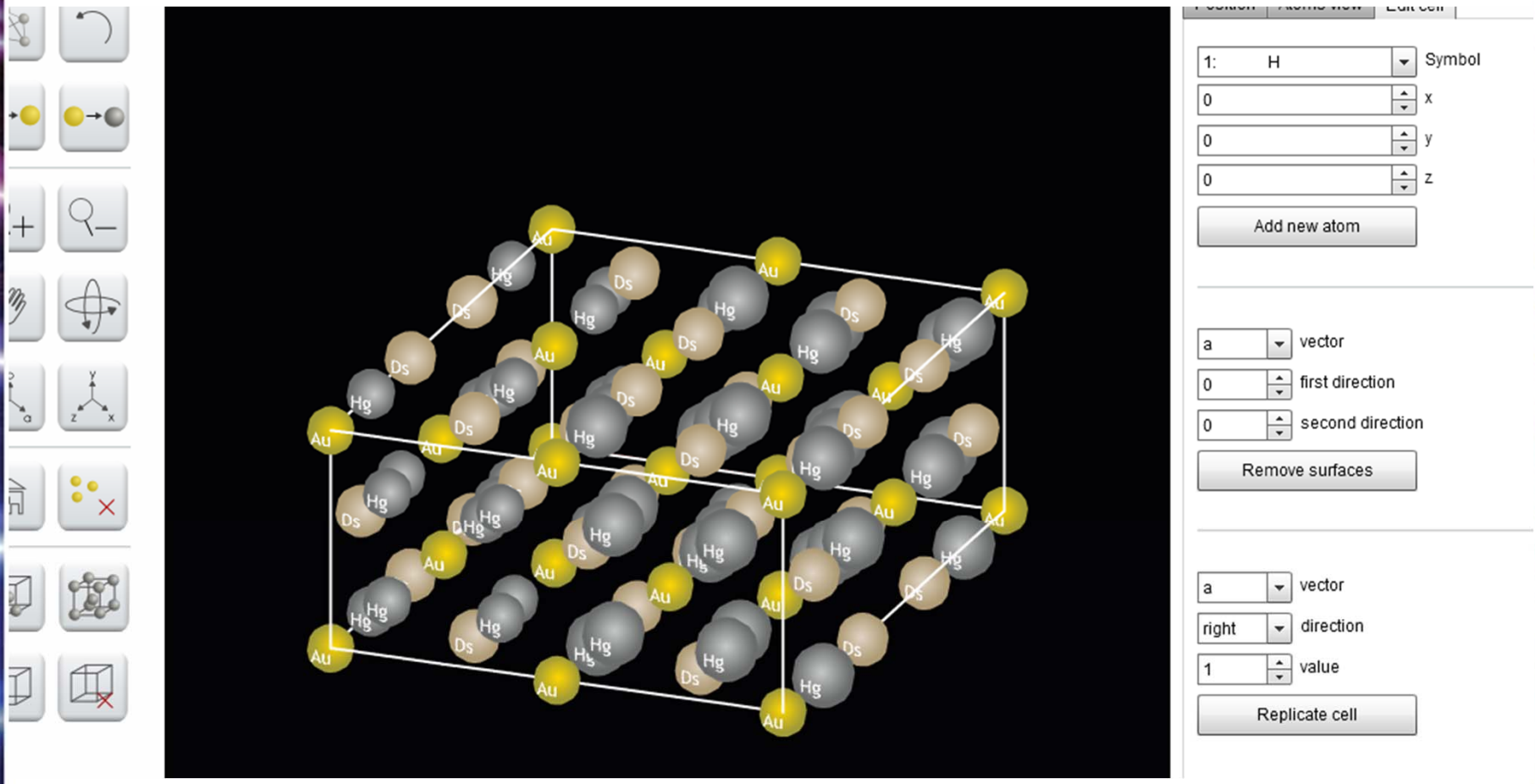
Nano-Science Gateway main view



NanoEditor

- Enables creation of nano structures, their visualization and modifications
- Consists of visual editor (further called NanoEditor) and interface that allows users to enter input data (further called NanoBuilder)
- NanoBuilder functionality covers:
  - creating crystal geometry using such parameters like: space group by its Hermann-Mauguin symbol, lattice vectors lengths, lattice angles, number of unit cells in each direction and telling whether unit cell should be found
  - Atoms could be added in a simple way, user can define their positions in Angstrom units
  - uses Spacegroup application from Elk software package (managed locally by the Vine itself and is made available through standard Job Management API)
  - generates output files which are used later in NanoEditor
- NanoEditor is a graphical tool that enables creating and editing super-cells and generating output files that can be further used in the Abinit package
  - cell replication
  - changing positions of certain atoms or groups of atoms
  - addition of atoms
  - defining the vacuum between cells
  - based on Papervision3D library

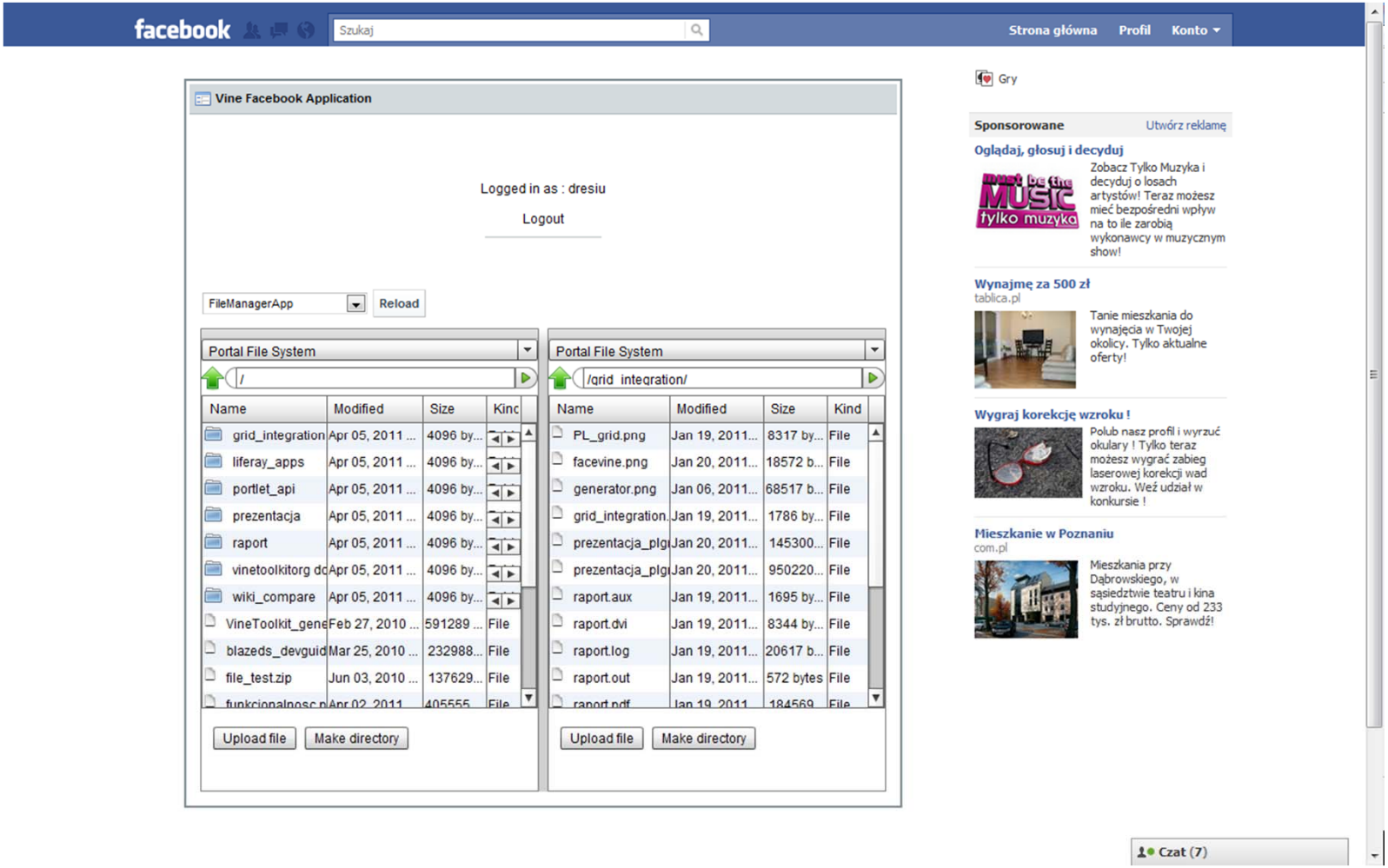
NanoEditor


1: H
Symbol
0
x
0
y
0
z
Add new atom
a
vector
0
first direction
0
second direction
Remove surfaces
a
vector
right
direction
1
value
Replicate cell

Towards modern web solutions

- Other Liferay based portals
- Social networks like Facebook
- Content aggregators, personalized web pages like iGoogle
- Vine web applications could be integrated into third part web infrastructures almost seamlessly
- We have tested Vine applications in a range of external web systems (starting from pure HTML pages, through Wiki, various CMS solutions, other instance of the Liferay, ending on Facebook and iGoogle)
- *RemoteVineGeneratorApp* - generate ready to use integration packages for various platforms (war packages)
- It is possible to set up Vine to automatically create an account for the new users (Single sign-up - SSU)
- Single sign-on (SSO) also supported
- SSO and SSU are implemented for Facebook and iGoogle currently
- Science Gateway components could be exposed in many places but controlled by central web server; other configurations possible

Facebook example



Future plans

- **PL-Grid National Grid Infrastructure** project
  - Main Liferay portal – production deployment, integration and support in 2011
  - Software validation through operational and security audits
  - More science gateways planned based on new end users requirements in domains like biotechnology or chemistry, etc.
  - Production SG deployments with QCG middleware developed by PSNC (although other middlewares also possible to use)
- Molecular Dynamics Gateway
  - Development continuation and support for new applications is planned (in case more end users will be involved)
- Beyond proxy certs - UNICORE SAML Assertion support in the future… (depends from ongoing actions and projects)
- Vine will be shipped with Serpens within Kepler release as an abstraction web service for grid infrastructures

Future plans

- Posible portals with QosCosGrid middleware support under the ongoing Infrastructure EU funded MAPPER project (Multiscale Applications on European e-Infrastructures) 2010-2013
  - closer collaboration with PRACE and EGI/EGI-InSPIRE partners possible
  - training sessions and workshops could be organized for PRACE and EGI users
- Production deployment of QCG middleware within infrastructural project PL-Grid on Polish NGI resources: PSNC, Cyfronet, TASK, (ICM maybe?)
- QCG production deployment during infrastructural MAPPER project (MoU with EGI, part of Task Force MAPPER-PRACE) – target sites LRZ (currently heavily tested), SARA
- Big impact from MAPPER communities from such domains: fusion, hydrology, physiology, nano-material science, computational biology
- Talks began with EMI, possible distribution of QCG middleware, Vine possibly could support EMI services

Any questions, comments or remarks are very welcome.

contact: dejw@man.poznan.pl

Vine Toolikt: http://vinetoolkit.org/

Vine users mailing list: vine-users@gforge.man.poznan.pl

PL-Grid: http://www.plgrid.pl/en/

Nano-Science Gateway: http://nano.man.poznan.pl

MAPPER: http://www.mapper-project.eu

QosCosGrid: http://www.qoscosgrid.org

Serpens: https://kepler-project.org/developers/interest-groups/distributed/serpens-suite-in-kepler