Plugin development – extensibility of UNICORE

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UNICORE projects at ICM

- **EUROGRID** (Nov. 2000 – Nov 2003)
  - ICM develops middleware for biomolecular applications,
  - ICM operates European grid for molecular biology

  - ICM deployed interoperable biomolecular applications

- **UNIGRIDS** (2004 – 2006)
  - ICM develops high level services (visualization, database access, access to remote instruments)
Unicore plugins

- UNICORE Client (5.3, 5.6)
- Example tasks:
  - **Quantum Chemistry**: Gaussian, TBDDFT
  - **Molecular Dynamics**: Amber, Gromos
- Plugins:
  - **Quantum Chemistry**: Gaussian, Gamess, CPMD (V. Huber FZJ)
  - **Molecular Dynamics**: AMBER
  - **BioInformatics**: BLAST (S. Haubold, TU Dresden)
  - **DataBase Access**: PDB Search, DBAccess
  - **Visualization**: SapphireVis, IADemo, IVis
  - **Broker**: Resource Broker (UoM)
  - **Other**: ListAllJobs, PluginLoaderPlugin
Gaussian98 plugin

Input preparation
reads existing input, recognizes keywords

Molecule coordinate editor
formats:
• XYZ
• Z-matrix
• text
Gaussian98 plugin

CPU time estimate based on known algorithm scaling $O(N^4)$

Check program availability
Gaussian Plugin

J. Pytliński, A. Nowiński
Amber plugin

Ł. Skorwider, J. Wypychowski

Panel for each group of options

Default options

Help window

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Flag for the removal of translational and rotational motion at the beginning of the simulation.

-0 The translational and rotational motion about the center of mass is not removed (default)
-1 The above motion is removed one time at the beginning of the simulation.
Amber plugin

Find parameter button
List All Jobs Plugin

<table>
<thead>
<tr>
<th>UseSite</th>
<th>VSite</th>
<th>Job name</th>
<th>Status</th>
<th>Date</th>
<th>ID</th>
</tr>
</thead>
<tbody>
<tr>
<td>UoM</td>
<td>O300_wren_aft</td>
<td>UNAVAILABLE</td>
<td>UNAVAILABLE</td>
<td>UNAVAILABLE</td>
<td>UNAVAILABLE</td>
</tr>
<tr>
<td>UoM</td>
<td>PS2_frik</td>
<td>UNAVAILABLE</td>
<td>UNAVAILABLE</td>
<td>UNAVAILABLE</td>
<td>UNAVAILABLE</td>
</tr>
<tr>
<td>UoM</td>
<td>soltest</td>
<td>UNAVAILABLE</td>
<td>UNAVAILABLE</td>
<td>UNAVAILABLE</td>
<td>UNAVAILABLE</td>
</tr>
<tr>
<td>Paral//ab</td>
<td>SGI_Origin2000</td>
<td>Environment_test_1</td>
<td>SUCCESSFUL</td>
<td>11-05 00:02:22</td>
<td>161d71f3</td>
</tr>
<tr>
<td>Paral//ab</td>
<td>SGI_Origin2000</td>
<td>Gaussian98_job</td>
<td>SUCCESSFUL</td>
<td>10-25 02:19:12</td>
<td>8fe7fff4</td>
</tr>
<tr>
<td>IDRIS-CNRS</td>
<td>IBM-SP3-tlon</td>
<td>New_Job1</td>
<td>NOT_SUCCESSFUL</td>
<td>11-01 20:10:02</td>
<td>8b3fe892</td>
</tr>
<tr>
<td>Paral//ab</td>
<td>SGI_Omyx2</td>
<td>New_Job1</td>
<td>NOT_SUCCESSFUL</td>
<td>11-01 20:08:59</td>
<td>8b3fe83c</td>
</tr>
<tr>
<td>FZJ</td>
<td>IBM44P-170_aft</td>
<td>UNAVAILABLE</td>
<td>UNAVAILABLE</td>
<td>UNAVAILABLE</td>
<td>UNAVAILABLE</td>
</tr>
<tr>
<td>ICM</td>
<td>tajfun</td>
<td>TOO SLOW</td>
<td>TOO SLOW</td>
<td>TOO SLOW</td>
<td>TOO SLOW</td>
</tr>
<tr>
<td>ICM</td>
<td>hydra</td>
<td>New_Job1</td>
<td>NOT_SUCCESSFUL</td>
<td>11-20 06:19:54</td>
<td>4543fb9f</td>
</tr>
</tbody>
</table>

[Image of the LAJ Window displaying a table of jobs with columns for UseSite, VSite, Job name, Status, Date, and ID.]

Running threads: 3

Last refresh time: Mon Nov 25 17:35:29 CET 2002

Show also control jobs

[Buttons: Refresh, Close, Show in JMC]
PluginLoader Plugin

K. Benedyczak

UNICORE Client

File Job Preparation Job Monitoring Settings Extensions Help

- Watch jobs
- Interactive visualisation
- List Jobs
- Plugin Loader
- Visit

Plugin Loader

Virtual site:
- stanislaw_IA
- stanislaw_main
- stanislaw_main_IVis
- stanislaw_noPBS

Available plugins on Vsite:
- LAJPlugin.jar
- gaussianPlugin.jar
- DBBrowserPlugin.jar
- DBAccessPlugin.jar
- sapphirePlugin.jar

Plugin properties

- Name: Gaussian Plugin
- Version: 2.2
- Date: 12.01.2004
- Description: Plugin for Gaussian quantum chemistry code. Allows for input preparation and output visualization

Download
ResourcesList plug-in

- List of resources
- Software resources
- Software resources can be filter
Visualizer Plugin
K. Benedyczak, A. Nowiński

Visualizer plugin file chooser

Task name: Visualizer1

Select files which you wish to fetch to workstation and visualize.

NOTE 1: Destination must be 'Local'

NOTE 2: Remember about dependencies (specified below files must exist before this task will...
Visualizer Plugin

K. Benedyczak, A. Nowiński
SapphireVis plugin

- Provides quick visualization for results files
- Allows quite advanced 2D visualization
- Easy in use
- Simple sample of sapphire library power
PDB search plugin

M. Wroński

Simple and advanced search

User can use different mirrors

The best one is selected (fastest answer)
PDB search plugin

User can use different mirrors

The best one is selected (fastest answer)
PDB search plugin

M. Wroński

Search results

Title: Crystal Structure Of Human Tyrosine-Protein Kinase C-Src, In Complex With Amp-Pnp

Compound: Mol_Id: 1; Molecule: Tyrosine-Protein Kinase Src; Chain: Null; Fragment: Residues 86-836, Containing Sh2, Sh3, Kinase 2 Domains and C-Terminal Tail; Synonym: C-Src, P60-Src; Ec: 2.7.1.112; Engineered: Yes; Biological Unit: Monomer

Authors: W. Xu, A. Doshi, M. Lei, M. J. Eck, S. C. Harrison

Exp. Method: X-ray Diffraction

Classification: Tyrosine-Protein Kinase

EC Number: 2.7.1.112

Source: Homo sapiens

Primary Citation: Xu, W., Doshi, A., Lei, M., Eck, M. J., Harrison, S. C.: Crystal Structures of C-Src Reveal New Features of its Autoinhibitory Mechanism Molecular Cell B pp.629 (1999) [Medline]

Deposition Date: 29-Dec-1998

Release Date: 22-Jul-1999
PDB search plugin

Visualization with external packages

Rasmol

JMV

Jmol

User-defined
Sequence search plugin

Search interface

M. Wroński
### Detailed view

**Sequence search plugin**

![Image of a detailed view window](image)

**Summary Information**

- **LOCUS**: XM_292775
- **DEFINITION**: Homo sapiens similar to ABC histo-blood group B transferase (LOC342885), mRNA.
- **ACCESSION**: XM_292775
- **VERSION**: XM_292775.2, GI:37552060
- **SOURCE**: Homo sapiens (human)
- **ORGANISM**: Homo sapiens
  - Eukaryota; Metasco; Chordata; Craniata; Vertebrata; Euteleostomi; Mammalia; Eutheria; Primates; Catarrhini; Hominidae; Homo.
- **COMMENT**: MODEL: REFSEQ: This record is predicted by automated computational analysis. This record is derived from an annotated genomic sequence (NT_011109) using gene prediction method: Gnomon.
- **Documentation**: of NCBI's Annotation Process

On Oct 7, 2003 this sequence version replaced gi:29741532.

**FEATURES**

- **Location/Qualifiers**
  - **source**: 1..951
    - /organism="Homo sapiens"
    - /mol_type="mRNA"
    - /db_xref="taxon:9605"

**Save**
Sequence search plugin

Simple visualization based on BIOJava
DBAccess Plugin

- Access to the SQL databases
  - MySQL
  - Postgress
  - SRB

- Results can be saved in the file

- XML output
FileConv Plugin

M. Wroński

![UNICORE Client](image)

**Task**
- **Task name**: New_FileConv5
- **XSLT processor**: XML::LibXML

<table>
<thead>
<tr>
<th>Source</th>
<th>Destination</th>
<th>Stylesheet</th>
</tr>
</thead>
<tbody>
<tr>
<td>n1</td>
<td>out1</td>
<td>DBAccess→Plain</td>
</tr>
<tr>
<td>n2</td>
<td>out2</td>
<td>DBAccess→Plain</td>
</tr>
</tbody>
</table>
Access to the external devices

- Advantech ADAM5000
- Deamon for the device running on the target system
- Management of the cluster hardware
Access to the external devices

- Thermometer connected through serial port to TSI server
- Daemon for the device running on the target system
- DeviceSteer Plugin
DeviceSteer

K. Benedyczak
DeviceSteer

K. Benedyczak
**IVis**

- **IVis concept**
  - data stream
  - performance
  - firewalls

  - Stream data through UNICORE Gateway using Gateway plugin
  - Simple authorization
  - Multiple clients can connect to the single visualization
  - IVis is available at SourceForge

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**UNICORE Client**

**UNICORE Gateway**

**IVis gateway (handler)**

**Vvis enabled NJS**

**NJS**

**NJS_IVis (IVis server)**

**UUDB**

**uspaces**

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K. Benedyczak, A. Nowiński
Plugin allows for easy files download from running job directory and visualization (or export to disk)
IVis – build-in visualization
Currently Amber job monitor is provided
Plain text file preview is available
Any ASCII data file can be interpreted
Other visualizations can be easily added, depending on requirements
IVis – build-in visualization

K. Nowiński

MolDyAna visualization

Reads streamed data
IVis performance

- **IVis tests**
  - Throughput is well acceptable
  - 2D and 3D visualization
  - Works with Amber, Gromos

100Mbit LAN, no routers

11Mbit Wi-Fi + LAN with 3 ro
Job submission.
For the job: MyScript8 on site: Warsaw get:

stdout

15:44:15 09/12 S Initial user incarnation is <unicore_demo/> Y
15:44:15 09/12 C Arrived at Warsaw
15:44:15 09/12 S Status is now READY
15:44:15 09/12 S Status is now EXECUTING. Message: Start processing of AJO
15:44:15 09/12 T Starting to execute
15:44:15 09/12 T Incarnating a Uspace
15:44:15 09/12 T AJO and Uspace initialised. Starting execution
15:44:15 09/12 T Starting child action
<MyScript8_ACTIONGROUP_1102603455028_17/596756d>
15:45:19 09/12 T Child action done
<MyScript8_ACTIONGROUP_1102603455028_17/596756d> with status <SUCCESSFUL>
15:45:19 09/12 T AJO execution finished, now clearing Uspace incarnation
15:45:19 09/12 S Status is now SUCCESSFUL
15:45:19 09/12 T Uspace cleared. Finishing
15:48:29 09/12 S RetrieveOutcome request from <EMAILADDRESS=kura@icm.edu.pl, CN=kura, OU=ICM, O=UW, L=Wa, ST=MA, C=PL>
15:48:29 09/12 T Complete Outcome (including incarnated data) will be sent to client
15:50:02 09/12 S RetrieveOutcome request from <EMAILADDRESS=kura@icm.edu.pl, CN=kura, OU=ICM, O=UW, L=Wa, ST=MA, C=PL>
15:50:02 09/12 T Complete Outcome (including incarnated data) will be sent to client
15:57:05 09/12 S RetrieveOutcome request from <EMAILADDRESS=kura@icm.edu.pl, CN=kura, OU=ICM, O=UW, L=Wa, ST=MA, C=PL>
15:57:05 09/12 T Complete Outcome (including incarnated data) will be sent to client

stderr

log
Adam2k GridBean

K. Benedyczak
GPE AppletClient

J. Jurkiewicz
GPE AppletClient

J. Jurkiewicz
GPE AppletClient

J. Jurkiewicz

![Image of a web page with a table showing job status and output]

<table>
<thead>
<tr>
<th>Action</th>
<th>Input</th>
<th>Output</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>blablablias</td>
<td>POVRay</td>
<td>SUCCESSFUL</td>
<td>Embedded Linux TSS</td>
</tr>
<tr>
<td>b1</td>
<td>POVRay</td>
<td>SUCCESSFUL</td>
<td>Embedded Linux TSS</td>
</tr>
<tr>
<td>pb2</td>
<td>POVRay</td>
<td>SUCCESSFUL</td>
<td>Embedded Linux TSS</td>
</tr>
<tr>
<td>present</td>
<td>POVRay</td>
<td>SUCCESSFUL</td>
<td>Embedded Linux TSS</td>
</tr>
<tr>
<td>pb3</td>
<td>POVRay</td>
<td>READY</td>
<td>Embedded Linux TSS</td>
</tr>
<tr>
<td>pb4</td>
<td>POVRay</td>
<td>SUCCESSFUL</td>
<td>Embedded Linux TSS</td>
</tr>
</tbody>
</table>
Lesson learned

- Plugin is a very good concept
- However....
  - development must be easier
  - configure rather than program
    - Amber, GenericPlugin
  - plugins too much depend on the UNICORE Client
  - UNICORE is a moving target
    - plugins are difficult to maintain
  - need for modularity and internal workflows
    - MetaPlugin
  - applications are changing
Plugin development Team

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- Aleksander Nowiński
- Jakub Jurkiewicz
- Jarosław Wypychowski