Computational Chemistry Cluster – EGEE-III Work Plan

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NA4 All Hands Meeting,
Paris, 9-10 June 2008

www.eu-egee.org

Partners

- ACC Cyfronet AGH
- University of Perugia
- CESNET
- KTH
- University of Innsbruck

Work Plan

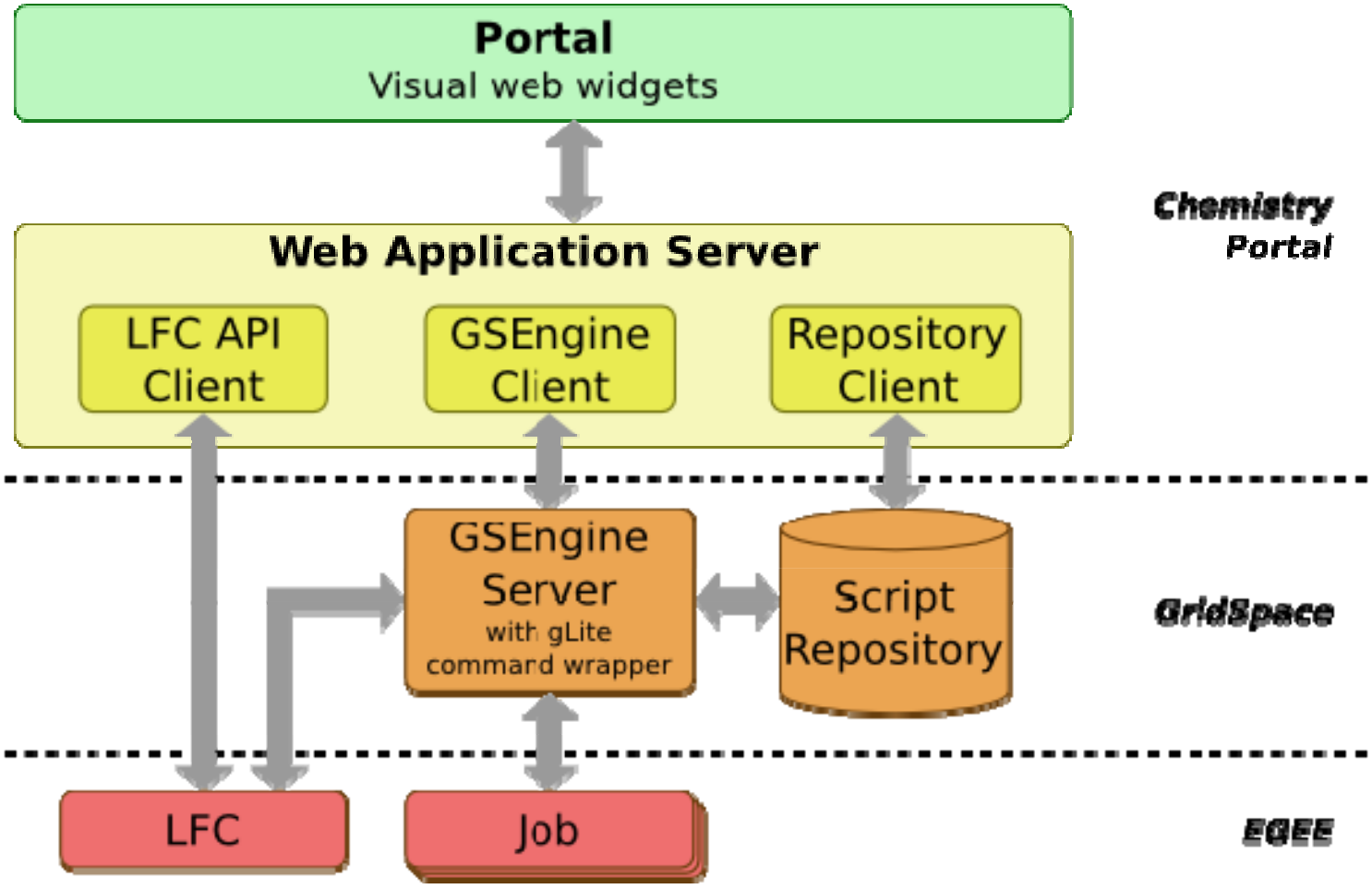
- Cluster Management 3PM M1-24
- Management of VOs supporting CC. users 4PM M1-24
- Extension of Charon GUI 5PM M1-12
- Extension of Wien2K workflow 5PM M1-12
- Development of ECCE port on gLite 5PM M1-12
- Development of grid license models 6PM M1-12
- Development web portal for chemists 30PM M1-24
- Development of grid port of parallel version of chemical software packages 8PM M1-24
- Expansion of the segment of EGEE Grid available for users from chemistry domain 4PM M13-24
- Execution efficiency testing 6PM M13-24
- First line support for users, training and dissemination 2PM M1-24

Elevator pitch

FOR researcher from computational chemistry domain, WHO want to use grid without changing their way of thinking and being distracted by technology. THIS computational environment IS a web portal with integrated tools, WHICH enable convenient and natural management of both computational process and experiment data on grid. COMPARING TO any other grid portal OUR PRODUCT is experiment-centric not grid-centric.

- **Goals:**
  - **Provide convenient user-data-centric environment for chemical computation using Grids**
  - **Build portal-like framework for quick application adaptation on grids that results with application- and data- oriented 'extensions' for specific application**

API details


Portal
Visual web widgets
Chemistry Portal
Web Application Server
LFC API Client
GSEngine Client
Repository Client
GSEngine Server
with gLite command wrapper
Script Repository
GridSpace
LFC
Job
EGEE

API details cont.

- The GUI layer will be implemented as a web application with the support of GWT (Google Web Toolkit) library. In order for the application to provide users with desired features the components underlying the web server (as depicted in the picture showed previously) need to deliver certain functionality described in the following list:
  - The LFC API Cient is used to manage the user data
  - GSEngine Client for application execution
  - Repository Client for application scripts storage


Editable Grid


Grid with Lo...

Grid with Re...


FieldSet


Multi Column


Load / Submit


Multiple Fie...


Form with Tab

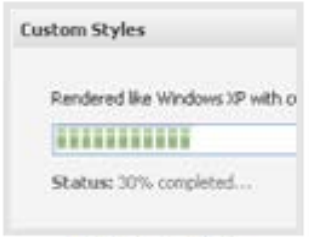

Form Grid Bi...

Dynamic Tabs

Bottom Tabs

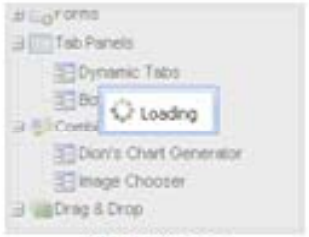

Dion's Chart...


Portal Demo



Progress Bar

Tooltips



Mask Demo


Image Chooser

Quantum dynamics engines of COMPCHEM for grid enabled molecular simulators

PARIS 9-10 – NA4 all hands meeting

Antonio Laganà

Department of Chemistry, University of Perugia, I

UNIPG MAIN TASKS

- SCIENCE: DEVELOP GRID EMPOWERED QUANTUM APPROACHES TO DESCRIBE THE DYNAMICS OF MOLECULAR SYSTEMS
- COLLABORATION: CREATE A VIRTUAL COMMUNITY IN MOLECULAR AND MATERIAL SCIENCES
- ORGANIZATION: IMPLEMENT AN ECONOMY OF THE VIRTUAL COMMUNITY

QDYN SCIENCE SUBTASKS

- Consolidate the atom diatom trajectory grid enabled molecular simulator GEMS
- Extend to 3D quantum calculations
- Carry out massive computational campaigns
- Extend the trajectory simulator to large sistems
- Introduce semiclassical corrections
- Implement quantum methods (TD,TI, MC,Prop)
- Assemble appropriate workflows

BY SIDE INTERESTS

- Structure programs as community services
- Develop a credit policy
- Push up user levels to the next layer

THE COMPCHEM APPROACH

1. USER
   PASSIVE : Runs other's programs
   ACTIVE: Implements at least one program for personal usage
2. SW PROVIDER (from this level one can earn credits)
   PASSIVE : Implements at least one program for other's usage
   ACTIVE: Management at least one implemented program for cooperative usage
3. GRID DEPLOYER
   PASSIVE : Confers to the infrastructure at least a small cluster of processors
   ACTIVE: Contributes to deploy and manage the structure
4. STAKEHOLDER: Takes part to the development and the management of the virtual organization

- **Further information at http://compchem.unipg.it**

NEXT ACTIVITIES

- Workshop at the International Conference on computational science and its applications to be held in Perugia (June 30 – July 3)
- Presentation of EGEE activities at the EUCO CC7 conference in Venice (Sept 12-15)
- Training School (Trieste Sept 15-18)

Wien2k on gLite
Status report EGEE III

Max Berger
Distributed and Parallel Systems Group (DPS)
University of Innsbruck
NA4 All Hands meeting, Orsay, Jun. 2008

Current Status

Transition EGEE II → III

- **Reduced effort in EGEE III**

Work in progress

- **Further optimization**
  - Worker model proved sucessful
  - Measured specific overheads
  - Auto-deployment was a large factor, could be reduced
  - Data Transfer is still a large factor, models are being explored

EGEE III Milestones

Future plans for EGEE III:

- **05 / 08 M0**
  - Project start
- **10 / 08 M1**
  - End of optimizations.
- **04 / 09, M2**
  - Clean up code,
  - Resolve distribution issues (e.g. licensing)
  - Provide end-user friendly package
  - End of our involvement in NA4

NA4 CESNET Activity

Computational Chemistry Plans

Jan Kmuníček

CESNET EGEE effort

NA4 EGEE activity

NA4 activity

- **CESNET involvement in NA4 (EGEE III)**
  - total **CESNET effort** for whole project duration **17 PMs**

    6 PMs clusters Computational Chemistry Cluster
    (with UIBK and CYFRONET)
  - personnel

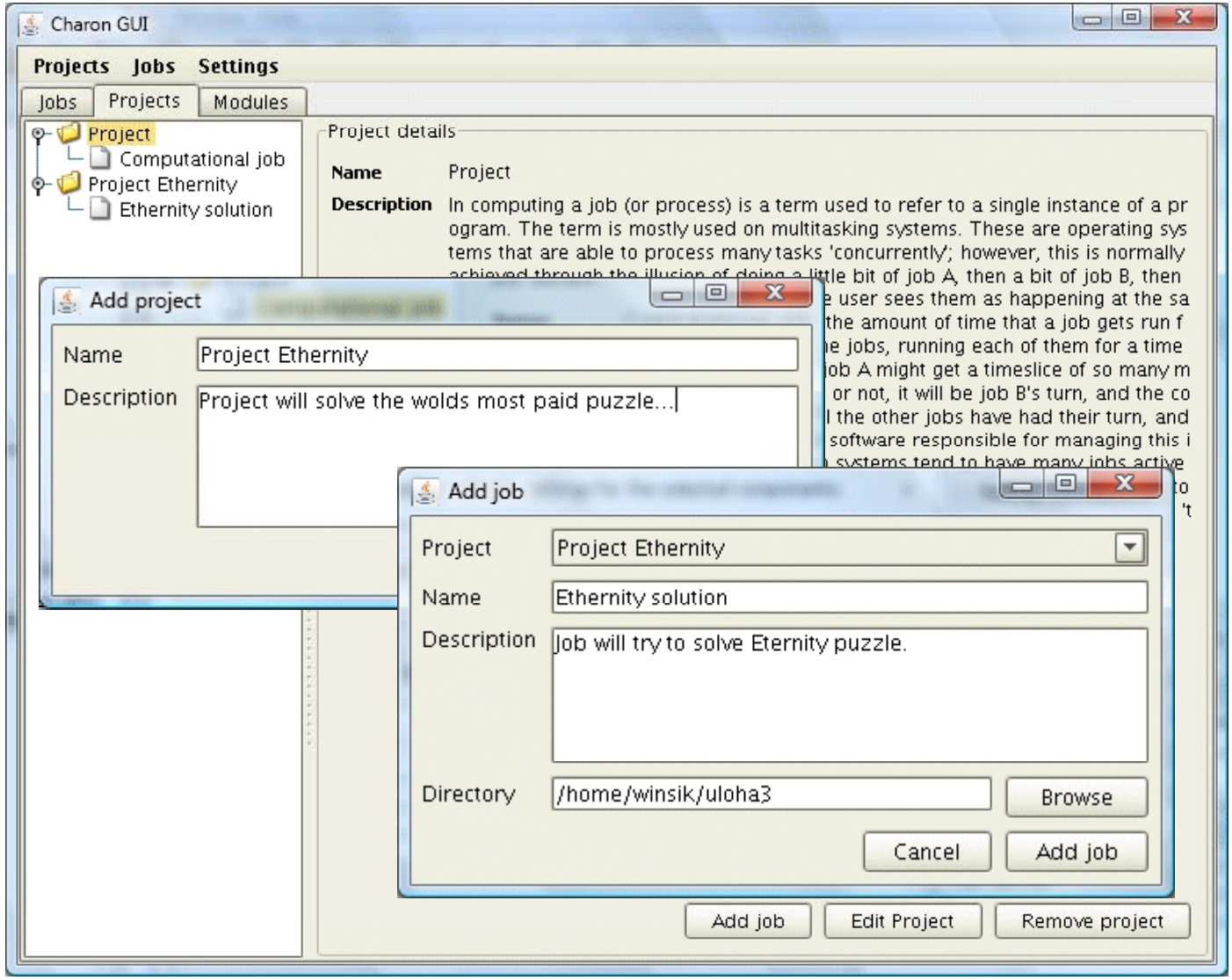
    Jan Kmunicek 6 PM (0.25 FTE)

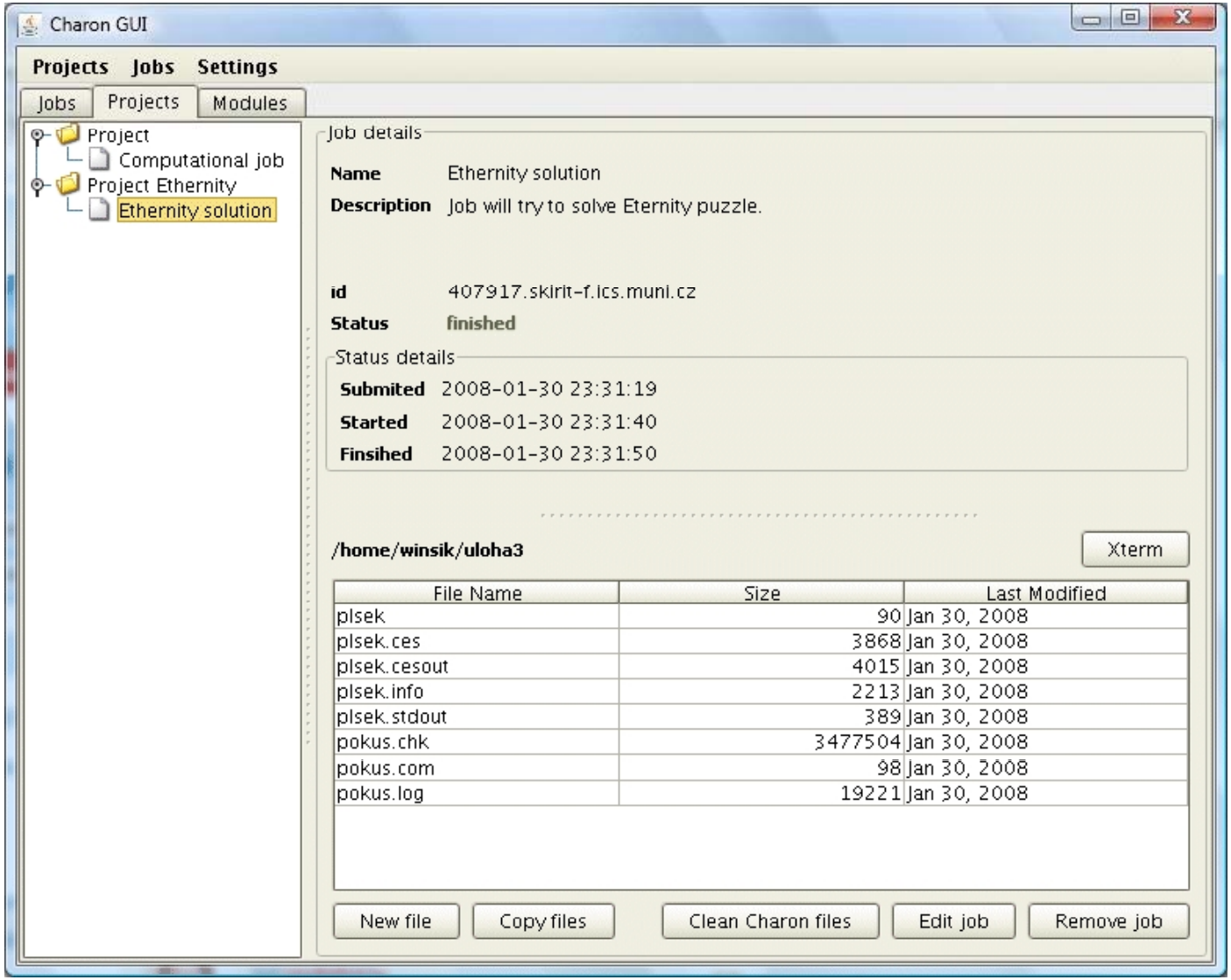
    new hired persons
    according to end users requirements and needs

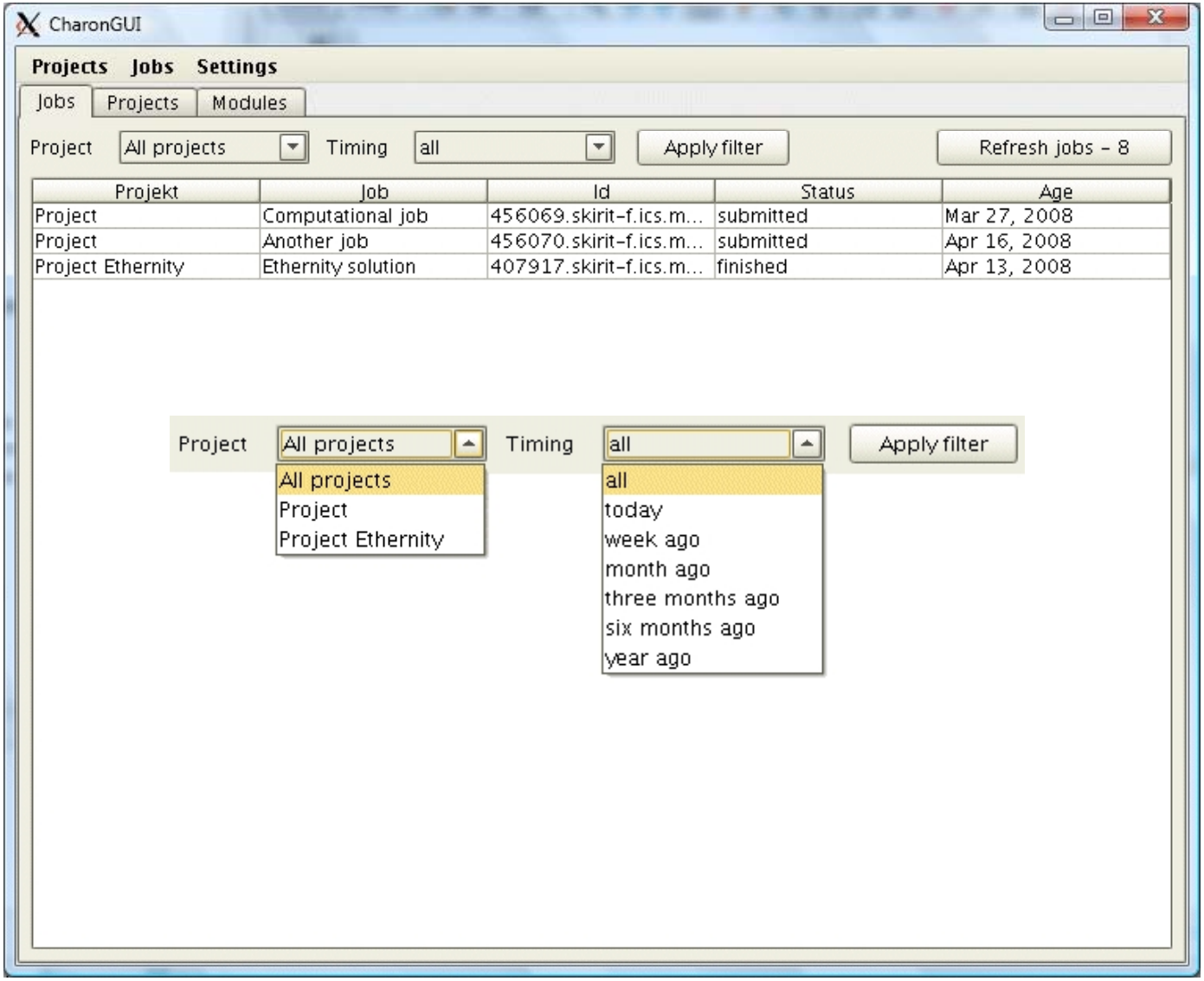
- **CESNET involvement in NA4 (EGEE III)**

  Computational Chemistry cluster tasks

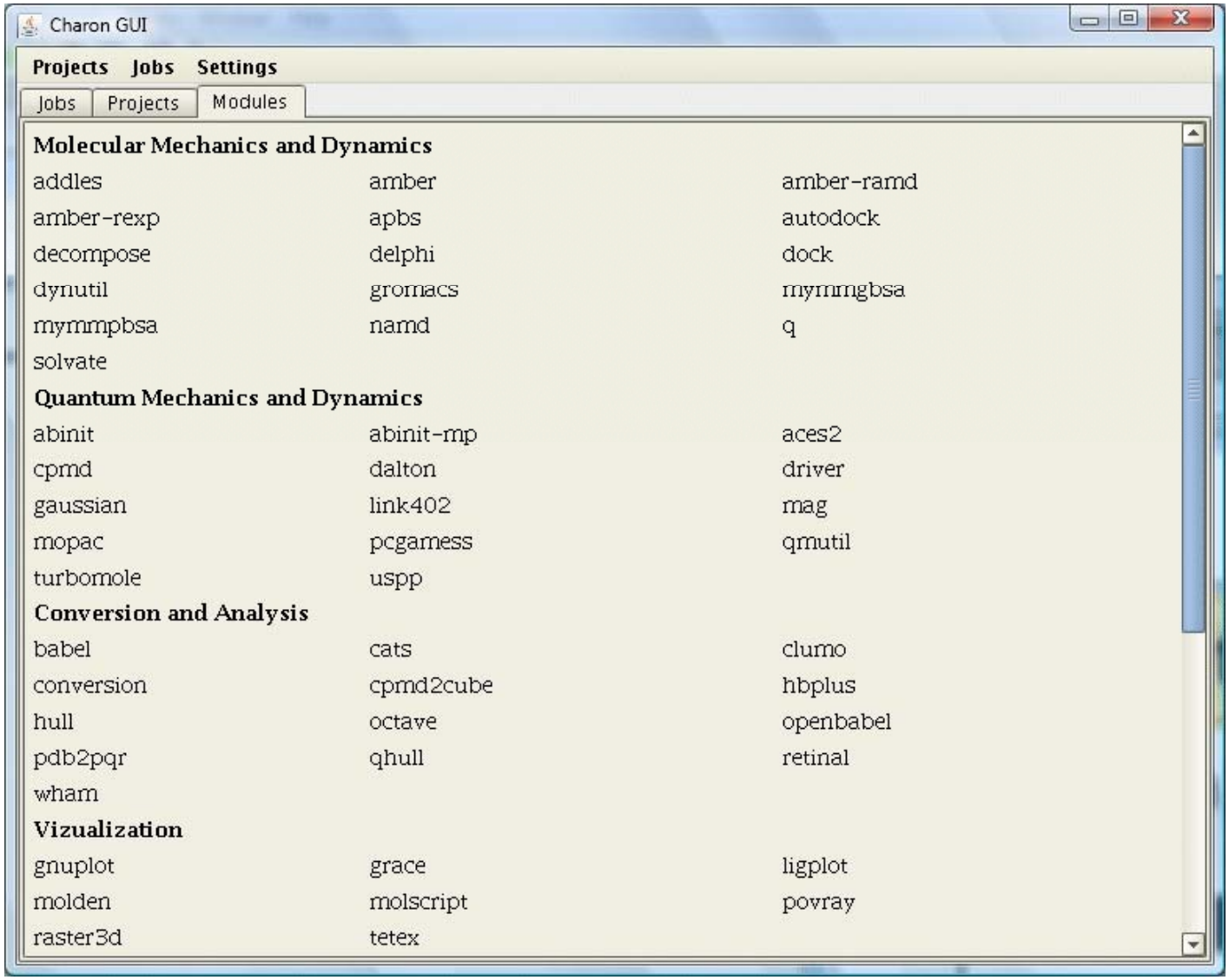
  - participation on development of reliable licensing model for utilization of commercial software packages
  - integration of computational chemistry software with (web) portals and/or provision of high level application dashboards (as Charon Extension Layer, CharonGUI, customized solutions …)
  - extension of available application portfolio (through packages currently being tested within Czech national grid environment/initiative)


Charon GUI
Projects Jobs Settings
Jobs Projects Modules
Project
Computational job
Project Ethernity
Ethernity solution
Project details
Name Project
Description In computing a job (or process) is a term used to refer to a single instance of a pr
ogram. The term is mostly used on multitasking systems. These are operating sys
tems that are able to process many tasks 'concurrently'; however, this is normally
Add project
Name Project Ethernity
Description Project will solve the wolds most paid puzzle...
Add job
Project Project Ethernity
Name Ethernity solution
Description Job will try to solve Eternity puzzle.
Directory /home/winsik/uloha3
Browse
Cancel
Add job
Add job
Edit Project
Remove project


Charon GUI
Projects Jobs Settings
Jobs Projects Modules
Project
Computational job
Project Ethernity
Ethernity solution
Job details
Name Ethernity solution
Description Job will try to solve Eternity puzzle.
id 407917.skirit-f.ics.muni.cz
Status finished
Status details
Submited 2008-01-30 23:31:19
Started 2008-01-30 23:31:40
Finsihed 2008-01-30 23:31:50
/home/winsik/uloha3
Xterm
File Name Size Last Modified
plsek 90 Jan 30, 2008
plsek.ces 3868 Jan 30, 2008
plsek.cesout 4015 Jan 30, 2008
plsek.info 2213 Jan 30, 2008
plsek.stdout 389 Jan 30, 2008
pokus.chk 3477504 Jan 30, 2008
pokus.com 98 Jan 30, 2008
pokus.log 19221 Jan 30, 2008
New file
Copy files
Clean Charon files
Edit job
Remove job


CharonGUI
Projects Jobs Settings
Jobs Projects Modules
Project All projects Timing all Apply filter Refresh jobs - 8
Projekt Job Id Status Age
Project Computational job 456069.skirit-f.ics.m... submitted Mar 27, 2008
Project Another job 456070.skirit-f.ics.m... submitted Apr 16, 2008
Project Ethernity Ethernity solution 407917.skirit-f.ics.m... finished Apr 13, 2008
Project All projects Timing all Apply filter
All projects
Project
Project Ethernity
all
today
week ago
month ago
three months ago
six months ago
year ago

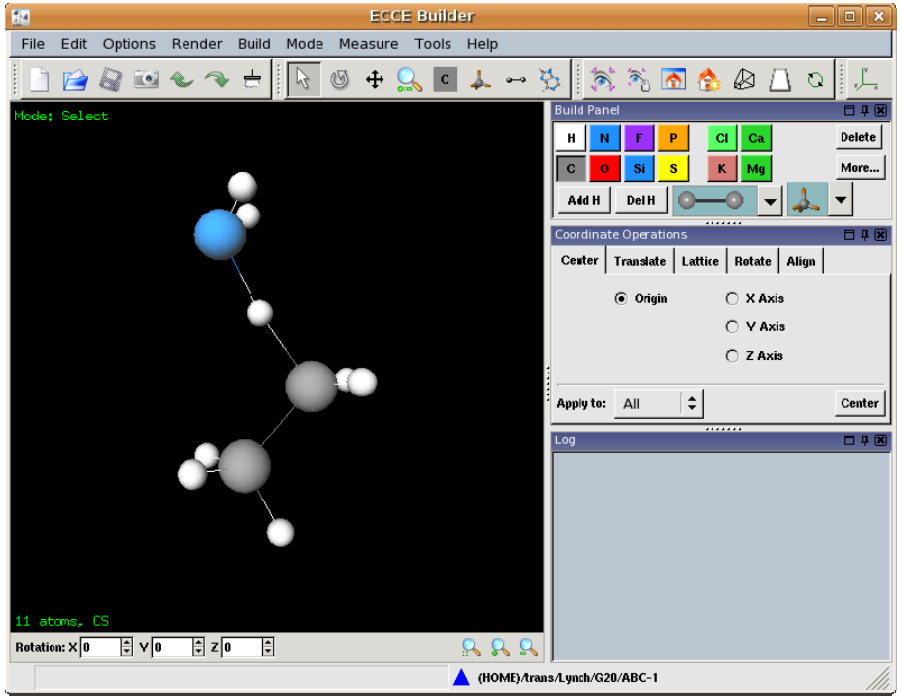
NA4 activity



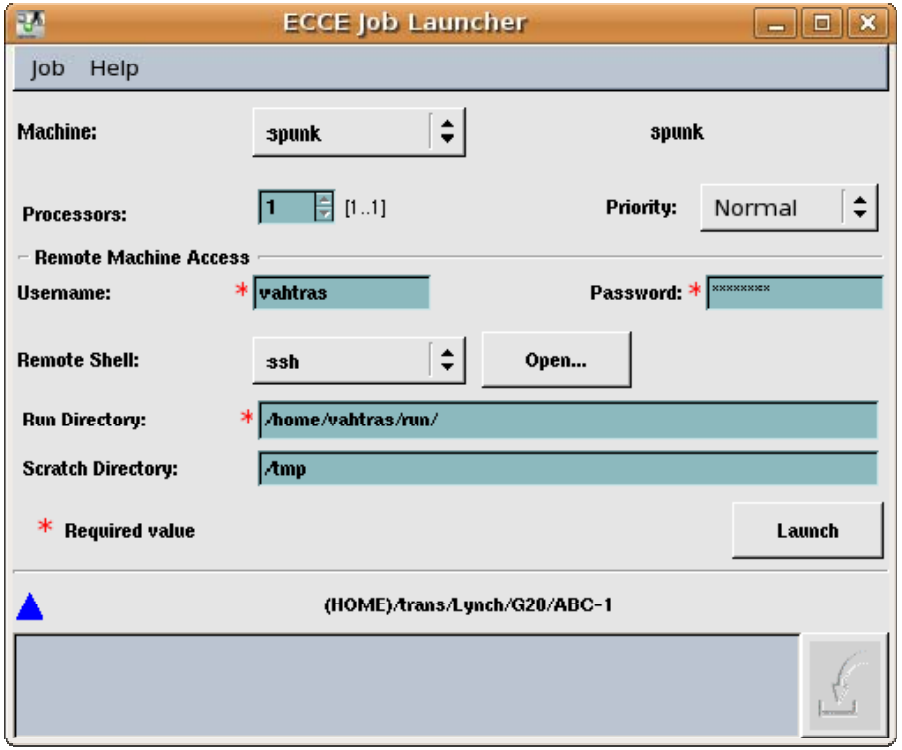
Ecce building blocks

- GUI **for building molecule, defining job type, choosing target cluster**
- Compute server**, local machine or computational clusters**
- Data server, **database storing computational results for all users**

Main panel



Builder



Launcher

Milestones

- Grid interface: setup glite/ARC interfaces for job submission to CE:s
- glite/ARC modules for monitoring status or running jobs
- Ecce database on SE:s

THANK YOU!

Questions?