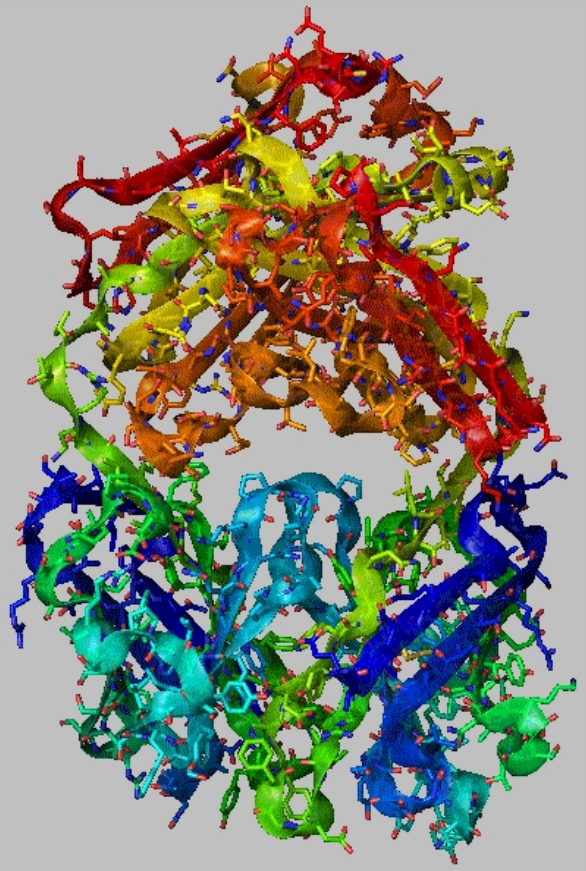
MetaCentrum

MetaCentrum – Czech grid e-Infrastructure

MetaCentrum

e-Infrastructure for solving structural biology research challenges



Jan Kmuníček, Martin Kuba

CESNET & ÚVT MU

meta.cesnet.cz

Content

- Structural biology
- Applications
- Support
- New services

Structural biology

- Engineering of (multi)-enzymatic structures
- QM/MM studies of catalysis
- Insight into the binding process
- Protein structure prediction
- Protein-protein docking
- Multidimensional parametric studies
- Genom/genome evolution analysis
- …

Structural biology

MetaCentrum – Czech grid e-Infrastructure

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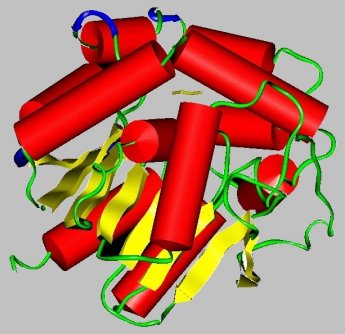
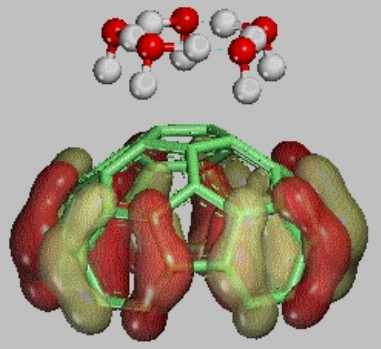
- **Computational chemistry**
  - § Amber — (bio)molecular simulations
  - § Gaussian — elektronic structure of molecules
  - § Gamess — ab-initio QM calculations
  - § Gromacs — molecular dynamics
  - § WIEN2k — elektronic structure of solids



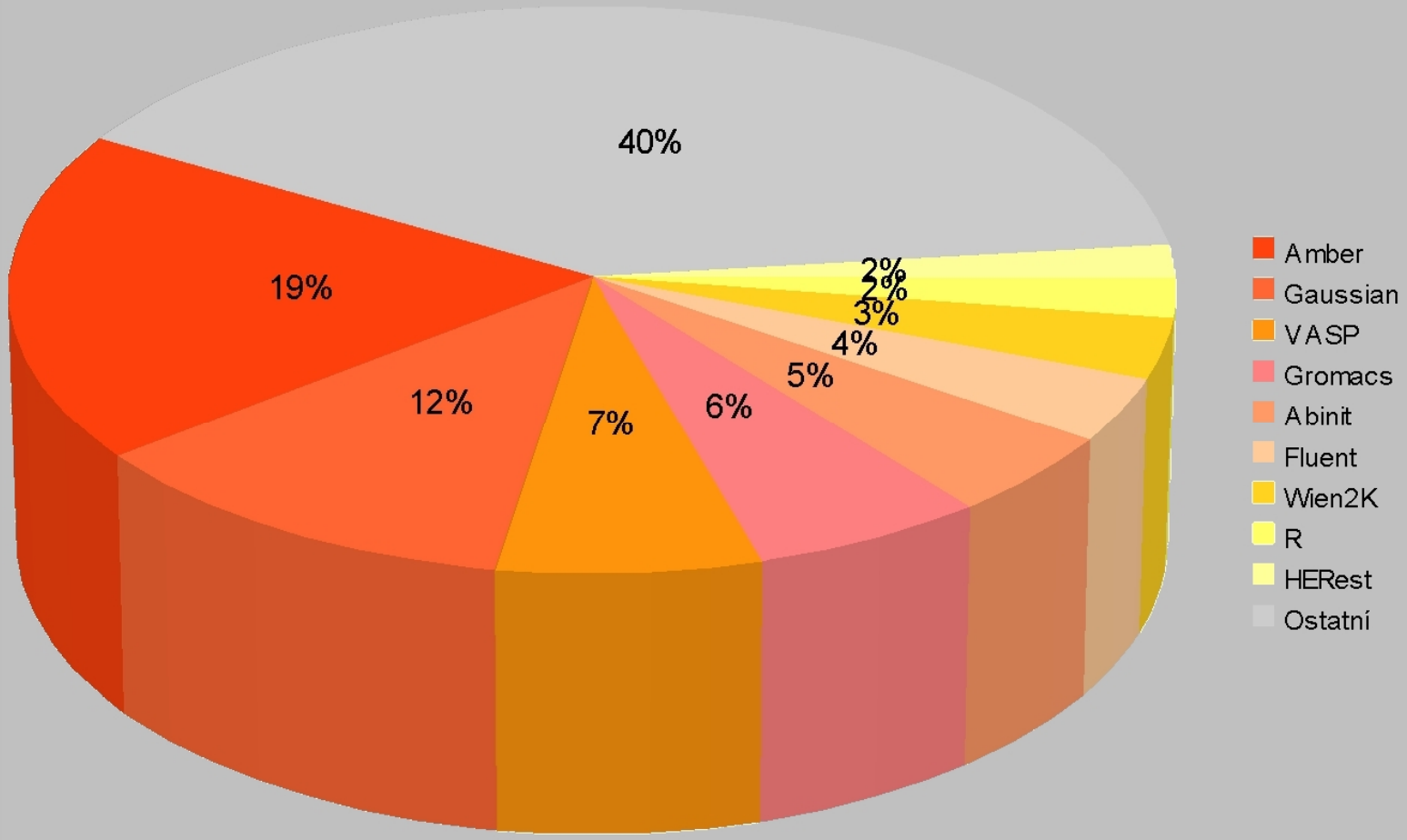
  - § *NAMD* — parallel dynamics of biomolecules
  - § *Tinker* — molecular mechanics/dynamics of biopolymers
  - § *VASP* — ab-initio QM molecular dynamics
  - § *Abinit* — elektronic structure of crystals

- **Structural biology/bioinformatics**
  - § X-Plor 3D structure of macromolecules
  - § Queen evaluation of NMR parameters
  - § MrBayes estimation of fylogeny
  - § CS-Rosetta generation of protein structures



- **User applications**
  - – installed by individual users themselves
    - § DL-POLY, Dalton, MPQC, ...

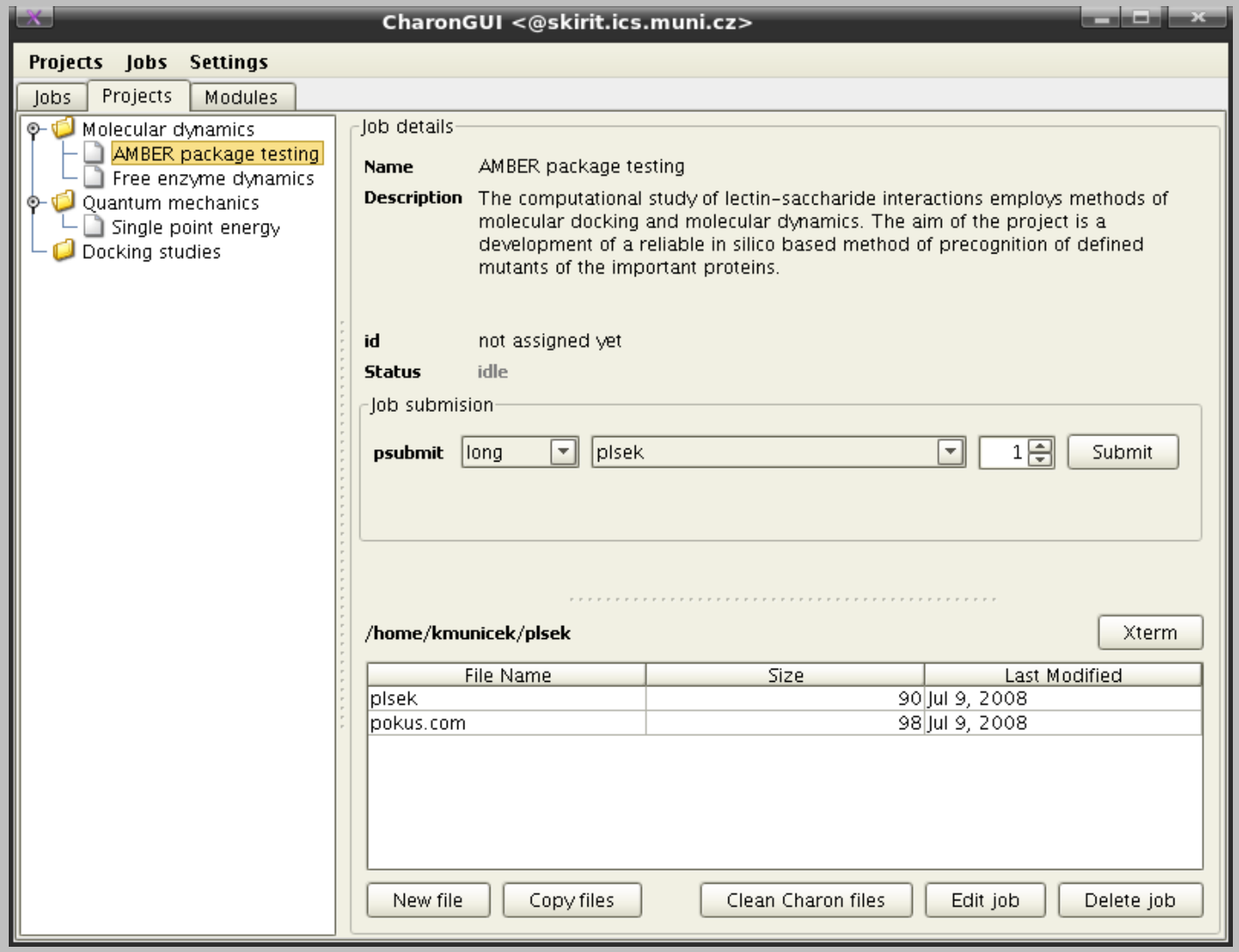
Computations time (user time, last year)

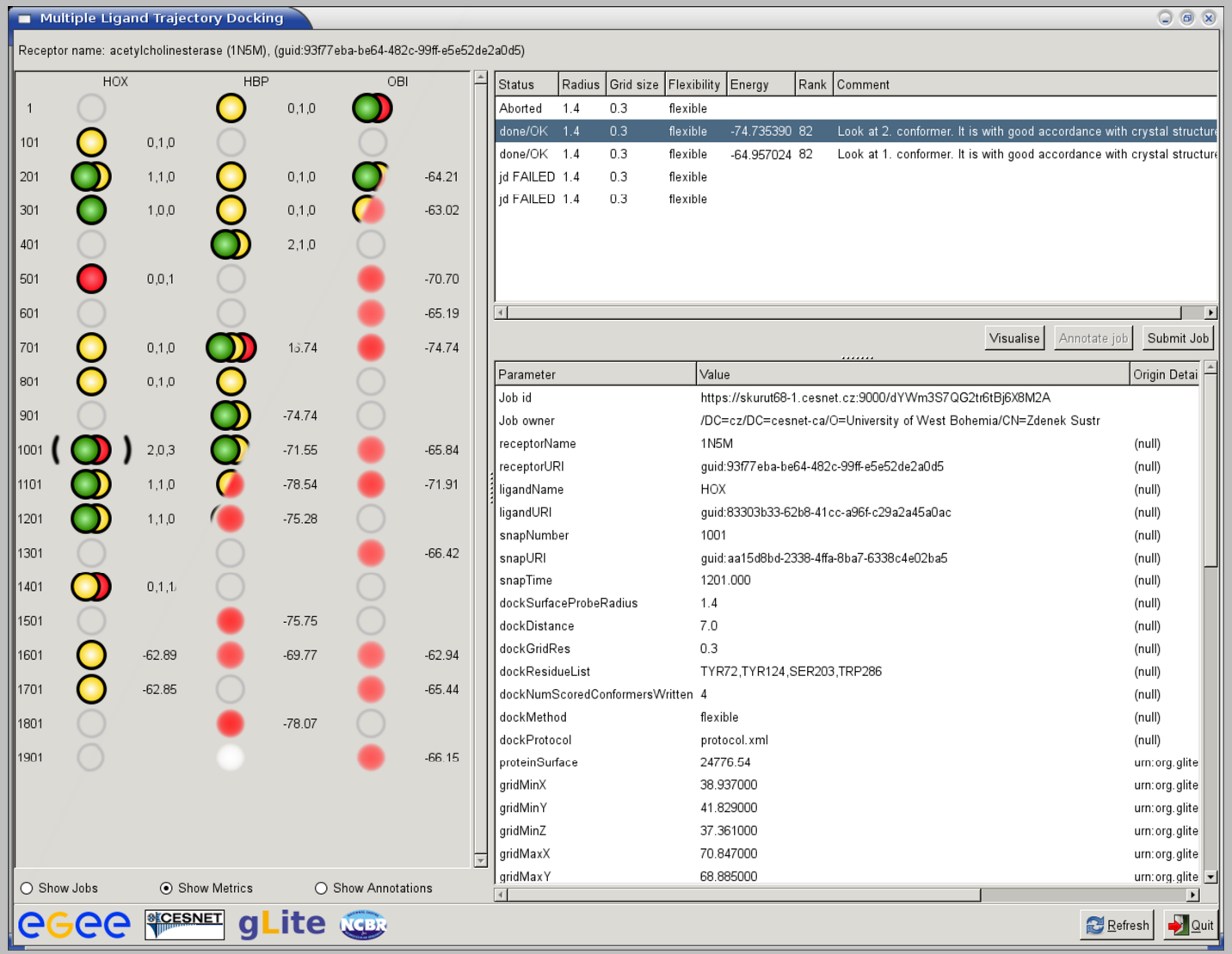


- **Basic concept**
  - end user utilizes an application software (OpenSource or commercial)
  - based on the request, according to licence and benefit for Meta users we help install and operate **user software**
  - MetaCentrum participation at costs needed for licenses purchase to cover (if possible) the whole MetaCentrum

Support

- **Forms of application support**
  - programs installation and update
  - request to RT
- **Development of user interfaces**
  - CharonGUI
- **Solutions „tailored to users needs“**
  - Multiple ligand trajectory docking
- **Testing of trial versions**
  - program ADF


CharonGUI <@skirit.ics.muni.cz>
Projects Jobs Settings
Jobs Projects Modules
Molecular dynamics
AMBER package testing
Free enzyme dynamics
Quantum mechanics
Single point energy
Docking studies
Job details
Name AMBER package testing
Description The computational study of lectin-saccharide interactions employs methods of molecular docking and molecular dynamics. The aim of the project is a development of a reliable in silico based method of precognition of defined mutants of the important proteins.
id not assigned yet
Status idle
Job submision
psubmit long plsek 1 Submit
/home/kmunicek/plsek
Xterm
File Name Size Last Modified
plsek 90 Jul 9, 2008
pokus.com 98 Jul 9, 2008
New file
Copy files
Clean Charon files
Edit job
Delete job


Multiple Ligand Trajectory Docking
Receptor name: acetylcholinesterase (1N5M), (guid:93f77eba-be64-482c-99ff-e5e52de2a0d5)
HOX
HBP
OBI
Status
Radius
Grid size
Flexibility
Energy
Rank
Comment
Aborted 1.4 0.3 flexible
done/OK 1.4 0.3 flexible -74.735390 82 Look at 2. conformer. It is with good accordance with crystal structur
done/OK 1.4 0.3 flexible -64.957024 82 Look at 1. conformer. It is with good accordance with crystal structure
jd FAILED 1.4 0.3 flexible
jd FAILED 1.4 0.3 flexible
Visualise
Annotate job
Submit Job
Parameter
Value
Origin Detai
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gridMaxX 70.847000 urn:org.glite
gridMaxY 68.885000 urn:org.glite
Show Jobs
Show Metrics
Show Annotations
Refresh
Quit

New services

- **Long-term aim**
  - **user driven infrastructure**
- **Means to reach the aim**
  - individualization of computational environment utilizing virtualization

- **Benefits of virtualization for users**
  - support for new types of utilization
  - support of preemption
    - § suspension of virtual machine to allow run of high priority computational jobs
  - user customizable environment
    - § up to own operation system
  - extremely easier resources management