CharonGUI Use Case: A Graphical Frontend to Key Services for Utilization of Grid Environments

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CESNET

www.eu-egee.org
• Charon System Evolution
• CharonGUI Use Case
  – CharonGUI Design
  – Look and Feel
  – Features
• Conclusions / Future Work
Charon System Evolution

- **Charon**
  - first attempt to ease daily Grid utilization
  - developed computational chemistry user group

- **Charon Extension Layer (CEL)**
  - further generalization of the concept
  - modified to support multiple underlying middleware
  - extensive expansion of supported/ported applications

- **CharonGUI**
  - next logical steps in the development
  - expected to attract “GUI-addicted” end users
  - maintain previous functionality
  - add new functions and useful services
• Charon
  – uniform and modular approach for (complex) computational jobs submission and management
  – generic system for use of application programs in the Grid environment (LCG/gLite middleware, PBSPro, OpenPBS, …)
Charon

No additional arguments are required – all information about job is stored in control files in job directory.
Charon System Evolution

- **Charon Extension Layer (CEL)**
  - application management
    - single/parallel execution without job script modification
  - job management
    - easy job submission, monitoring, and result retrieving

![Diagram of Charon System Evolution]

- CEL
  - charon system
    - job management
  - module system – software management
  - software repository
  - app 2, app 3, app 4, app 5, ........
  - batch system, grid middleware
  - user
CharonGUI Design

- Multiplatform concept
- Support for distinct grids
- Preservation of job life cycle characteristics
- Intuitive and user-friendly interface
- Multilingual support
## Look and Feel

### Molecular Mechanics and Dynamics
- addies
- amber
- amber-reexp
- apbs
- decompose
- delphi
- dynutil
- gromacs
- myrmypbsa
- namd
- solvate

### Quantum Mechanics and Dynamics
- abinit
- abinit-mop
- cpmd
- dalton
- gaussian
- link402
- mopac
- pgamess
- turbomole
- uspp

### Conversion and Analysis
- bebel
- conversion
- cpmd2cube
- hull
- octave
- pdb2pqr
- qhull
- wham

### Visualization
- grgroup
- grace
- molden
- molscript
- raster3d
- tetex
- Job files management
- Categorization of computational projects/jobs
- Checking status of multiple jobs
- Comfortable jobs submission

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<tr>
<th>File Name</th>
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<tr>
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<td>ookus.com</td>
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</table>
• Job files management
• Categorization of computational projects/jobs
• Checking status of multiple jobs
• Comfortable jobs submission
### Features

- Job files management
- Categorization of computational projects/jobs
- Checking status of multiple jobs
- Comfortable jobs submission

<table>
<thead>
<tr>
<th>Project</th>
<th>Job</th>
<th>Id</th>
<th>Status</th>
<th>Age</th>
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<tbody>
<tr>
<td>Molecular dynamics</td>
<td>AMBER package testing</td>
<td></td>
<td>idle</td>
<td>Oct 23, 2008</td>
</tr>
<tr>
<td>Molecular dynamics</td>
<td>Free enzyme dynamics</td>
<td>293972.skirt-f.lcs.mun...</td>
<td>finished</td>
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<tr>
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<td>Single point energy</td>
<td>488794.skirt-f.lcs.mun...</td>
<td>finished</td>
<td>Oct 23, 2008</td>
</tr>
</tbody>
</table>

### Project Selector

- All projects
- Project 1
- Project 2
- Project 3
Features

- Job files management
- Categorization of computational projects/jobs
- Checking status of multiple jobs
- Comfortable jobs submission
Individual job details and management

CharonGUI <@skirit.ics.muni.cz>

Projects Jobs Settings

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 submission

psubmit:
- long  
- pisek

/home/kmunicek/pisek

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<tr>
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<tr>
<td>pokus.com</td>
<td>98 Jul 9, 2008</td>
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Individual job details and management

**Description**
The computational study of lectin-saccharide interactions employs methods of molecular docking and molecular dynamics. The aim of the project is the development of a reliable in silico based method of recognition of defined mutants of the important proteins.

**Status**
**submitted**

**Submitted**
2008-10-23 11:27:48

**Files**

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</tr>
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</table>

**Files**

- pisek
- pisek.cs
- pisek.info
- pisek.com
Individual job details and management

CharonGUI

- **Projects**: Molecular dynamics, AMBER package testing, Free enzyme dynamics, Quantum mechanics, Single point energy, Docking studies

- **Jobs**:
  - **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**: 547732.skirit-ics.muni.cz
  - **Status**: running
  - **Submitted**: 2008-10-23 11:27:48
  - **Started**: 2008-10-23 11:28:03
  - **Finished**: 

- **Files**:
  - | File Name   | Size       | Last Modified |
  - |-------------|------------|---------------|
  - | psek        | 2.07 MB    | 90 Jul 9, 2008|
  - | pokus.com   | 98 B       | 9 Jul 9, 2008  |

- **Tools**: New file, Copy files, Clean Charon files, Edit job, Delete job
Individual job details and management

- **Project:** Molecular dynamics
- **Subproject:** AMBER package testing

**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.

**Status:** finished

**Execution:**
- **Submitted:** 2008-10-23 11:27:48
- **Started:** 2008-10-23 11:28:03
- **Finished:** 2008-10-23 11:28:25

**Files:**

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<tr>
<td>pokus.log</td>
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<td>19065 Oct 23, 2008</td>
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Individual job details and management

- File management
- Input files modification
- Xterm invocation
- Control files cleaning
- Job submit
- Job monitoring
- Results retrieval

EGEE-III INFSO-RI-222667
GCCP 2008, Bratislava, Slovakia
Individual job details and management

The electronic state is 1-SGO.
Alpha occ. eigenvalues -- -0.59884
Alpha virt. eigenvalues -- 0.24111 0.76997 1.41765
Condensed to atoms (all electrons):

 Mulliken atomic charges:
  1 H  0.000000
  2 H  0.000000
Sum of Mulliken charges= 0.00000
Atomic charges with hydrogens summed into heavy atoms:
  1 H  0.000000
  2 H  0.000000
Sum of Mulliken charges= 0.00000
Electronic spatial extent (au): <R**2>= 5.1665
Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):
X= 0.0000 Y= 0.0000 Z= 0.0000 Tot= 0.0000

"A LITTLE BIT GOES A LONG WAY"
D.S. MULLIKEN AS QUOTED BY K. DAHLENDREK

Job cpu time: 0 days 0 hours 0 minutes 12.0 seconds.
File lengths (MBytes): RWF= 11 Int= 0 DZF= 0 C1
Normal termination of Gaussian 03 at Thu Oct 23 11:28:24 2008
### Jobs filtering

The image shows a screenshot of a jobs filtering interface. The interface is divided into sections for Projects, Jobs, and Settings.

#### Projects
- **Molecular dynamics**
- **Quantum mechanics**

#### Jobs
- **AMBER package testing**
- **Free enzyme dynamics**
- **Single point energy**

#### Details
- **Project**: AMBER package testing
- **Id**: 547732.skirit.ics.muni..finished
- **Status**: finished
- **Age**: Oct 23, 2008

- **Project**: Free enzyme dynamics
- **Id**: 293972.skirit.ics.muni..finished
- **Status**: finished
- **Age**: Oct 23, 2008

- **Project**: Single point energy
- **Id**: 488791.skirit.ics.muni..finished
- **Status**: finished
- **Age**: Oct 23, 2008
Dropdown menu overview

The computational study of lectin-saccharide interactions employs methods of molecular docking and molecular dynamics. The aim of the project is the development of a reliable in silico based method of precognition of defined mutants of the important proteins.

Details:
- AMBER package testing
- Submitted: 2008-10-23 11:27:48
- Started: 2008-10-23 11:28:03
- Finished: 2008-10-23 11:28:25

Files:
- /home/kmunicek/psek

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Skins and languages

CharonGUI

Projects: Jobs
Settings

Themes:
- Molecular dynamics
- Free enzyme dynamics
- Quantum mechanics
- Single point energy
- Docking studies

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 pretargeting of defined mutants of the important proteins.

Status:
- Submitted: 2008-10-23 11:27:46
- Started: 2008-10-23 11:28:03
- Finished: 2008-10-23 11:28:23

Files:

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EGEE-III INFSO-RI-222667

GCCP 2008, Bratislava, Slovakia
• CharonGUI is Java-based application

• Current version runs at specific server
  – dedicated frontend/user interface to individual VOs
  – JRE-1.6.0 is the only prerequisite on server side

• Display on remote X-server
  – Linux, MS Windows with X-Window emulator

• Implemented functions
  – available in graphical interface itself and in dropdown menu
  – personalization of user settings (last project, …)
GUI over CLI Added Values

• Management of laboratory projects
  – allowing complete projects and jobs manipulation

• Exhaustive jobs overview and jobs filtering
  – based on job state, time period, project assignment, job IDs

• Invocation of Xterm for further analysis

• Advanced features
  – internationalization (languages)
  – support for visual skins
Conclusions

• **Drawbacks and issues**
  – latency
  – reading the console output (discovered issues to be fixed)

• **Deployment**
  – METACentrum (Czech NGI - National Grid Initiative)
  – VOCE (Virtual Organization for Central Europe)

• **Promotion outside Europe**
  – EUAsiaGRID project
Future Work

- Remote client version
- Extension of supported virtual organizations
- Multiple project hierarchy
- Configuration and installation tool
- Interactive list of application modules including links to on-line documentation