Graphical User Interface for Charon Extension Layer System and Application Dashboards

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CESNET NA4 effort
• Charon Extension Layer approach
• Charon GUI status and overview
• Application dashboards
• Current development plans
• Conclusions
Why Charon Extension Layer (CEL)?

- many various batch systems & scheduling components used in grid environment
- each batch system has unique tools and different philosophy of its utilization
- LCG/gLite provided tools are quite raw and simple
- many additional tasks to use computer resources properly
• **Application management**
  – single/parallel execution without job script modification

• **Job management**
  – easy job submission, monitoring, and result retrieving
• Typical job flow

[myjob]$ psubmit gilda test1  
submit job

[myjob]$ pinfo  
monitor job

[myjob]$ psync  
get results

No additional arguments are required – all information about job is stored in control files in job directory.
• **Graphical interface for Charon system**
  – offers simple and intuitive interface to predefined set of options in graphical, highly usable and reliable way
  – removes the need to memorize CLI commands

• **Basic cornerstones**
  – Charon GUI retains *simplicity/usability*
  – Charon GUI allows access to all *key functionalities*
  – adds a log of jobs and projects to which they belong
Technical details

- Charon GUI 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 through graphical
  interface itself as well in dropdown menu
- personalization of user settings (last project, …)
• **Complete list of features**
  
  - **key Charon Extension Layer functionality**
    - submit a job, monitor the job, retrieve results
    - exploration of available application modules
  
  - **added values of graphical interface**
    - **management of laboratory projects** allowing complete projects and jobs manipulation (add, remove, edit)
    - 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, support for skins
Molecular dynamics

AMBER package testing
Free enzyme dynamics
Enzyme plus ligand
Equilibration
Production run

Quantum mechanics
Ligand geometry optimization
Charges calculation
Single point energy 1
Single point energy 2

Docking studies
AutoDock
DOCK
FlexiO

Project details

Name: Molecular dynamics

Description: Interaction between large biomolecules and smaller bio-active ligands lies on the foundation of many biological properties and is of huge interest in the bio-molecular and pharmaceutical research. The role of the ligand is to influence the reaction that occurs in an active site of a biomolecule. The interaction is usually studied using multiple ligand trajectory docking, a computationally intensive process aimed to find energetically favorable orientation of the ligand within an active site.

The search is done on snapshots taken from the molecular dynamics trajectory describing the dynamic behavior of the biomolecule. For each snapshot and ligand the best position of the ligand is calculated, yielding a matrix containing energies of snapshot/ligand interactions. The minima correspond to the most favorable ligands and provide insight into the specific shape of the biomolecule.

The concrete problem shown in the demo deals with one Zins acetylcholinesterase trajectory and 5 ligands, requiring some 6000 CPU hours on an average compute server. A realistic studies use more and longer trajectories (tens ns) and higher number of potential ligands (tens to hundreds).

Performing such computation is infeasible without the Grid infrastructure. Also, managing its results is a non-trivial problem, unreadable without semi-automatic support tools. A sophisticated job submission system coupled with a community-wide provenance of already run jobs is a necessary prerequisite.
Adding new project / job

- **Add project**
  - Name: Computational chemistry
  - Description: Whatever study we would like to perform

- **Add job**
  - Project: Molecular dynamics
  - Name: Individual computational job
  - Description: Details description follows here

- **Open**
  - Look In: kmuricek
  - Directory: 
    - aas
    - bc
    - cel-gui
    - JDL Infos
    - papers
    - plsek
    - plsek2
    - plsek3
    - scb
  - File Name: /home/kmuricek
  - Files of Type: All Files
Individual job details and management

![Charon GUI window showing job details and management interface, focused on a job with the status 'idle' and the identifier 'not assigned yet'.]
Individual job details and management

![Screenshot of the Charon GUI interface showing individual job details. The highlighted job details include:
- **Name**: Enzyme plus ligand
- **Description**: MD performed on the complete biomolecular system
- **ID**: 3780001
- **Status**: running

The status details indicate:
- **Submitted**: 2007-11-30 20:39:02
- **Started**: 2007-11-30 20:39:37
- **Finished**: [status bar]

The bottom section of the GUI shows a file directory with various files, including:
- `plsek`
- `plsek.ces`
- `plsek.info`
- `plsek.com`

File sizes and last modified dates are also displayed.]}
Individual job details and management

Job details:
- Name: Enzyme plus ligand
- Description: MD performed on the complete biomolecular system
- id: 378001.skirt-files.muni.cz
- Status: finished
- Status details: finished

Submitted: 2007-11-30 20:39:02

/home/kmunicek/plsek3

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File management
Input files modification
Xterm invocation
Job control files cleaning

Job submit
Job monitoring
Results retrieval
Individual job details and management

Computational Chemistry Workshop, LAL Orsay, Paris
### Jobs filtering

#### Task project | Task name | Status
---|---|---
project | AMBER package testing | idle
project | Free enzyme dynamics | idle
project | Enzyme plus ligand | finished
project | Equilibration | idle
project | Production run | idle
project | Ligand geometry optimization | idle
project | Charges calculation | idle
project | Single point energy 1 | idle
project | Single point energy 2 | idle
project | AutoDock | idle
project | DOCK | idle
project | FlexX | idle
Dropdown menu overview
Multiple ligand trajectory docking

- interactions between large biomolecules and smaller bio-active ligands
  - lies on the foundation of many biological properties
  - interest in the biomolecular/pharmaceutical research
- interactions studied through a process called docking
  - aims to find energetically favorable orientation of the ligand within an active site of a biomolecule
• Introduction to the application
  – search is done on snapshots taken from molecular dynamic trajectory describing dynamic behavior of a biomolecule and a set of candidate ligands
  – such computation is *infeasible without Grid infrastructure*
  – Grid environment serves for
    performing required computationsCharon system
    management of resultsprovenance service
• Biomolecular aspects of chemical weapons
  – many organophosphate nerve agents
  – interference with the signaling system used by the nervous system
  – these compounds inhibit acetylcholinesterase (AChE) essential chemical that breaks down nerve signals between nerve cells
  – looking for universal reactivator able to liberate AChE when it is poisoned by the nerve paralytic compounds
• **Added Value for Application Experts**
  - GUI application for solving generic biomolecular parametric jobs
  - User application metrics evaluation based on targeted parameters
  - Potential extension for biomedical screening
  - Effective collaboration among researchers
  - Computational jobs manipulation (input modification, jobs resubmission)
  - Targeted search & selection of desired jobs (finished / non-finished, aborted)
  - Modular application specific plugins for results presentation (e.g. visualization)
The application supports selection of subsets of both trajectory snapshots and specific ligands, queries JP, and displays a **2D array of finished Grid jobs matching the criteria**.

3 views on the job array are supported: application-specific metrics of the job results, the user annotations, and the job status in Grid middleware.

Summary of jobs in a selected array cell.

Results of the selected job can be later examined in details, including three dimensional visualization of emerging complex 3D structures.

List of detailed information about selected job as gathered by JP service.
Current development plans

- Charon GUI features for implementation
  - core development
    - extension of supported virtual organization
    - remote client version
  - further enhancements
    - incorporation of subprojects
    - interactive list of application modules including links to Charon on-line documentation
Conclusions

• Modular base of Charon system allows extensibility
  
  – Charon GUI has been developed and its moreless ready for production release
  
  – Charon system itself can serves as building block for incorporation into even higher customized applications (dashboards or workbenches)