

Charon – Hands on Session

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The logo consists of three overlapping squares: a purple one at the top, a blue one on the left, and a white one at the bottom right, all with thin black outlines.

UI Information

User Interfaces for GILDA VO

- glite-tutor.ct.infn.it*
- glite-tutor2.ct.infn.it*

***) Both machines share the same home directories.**

Accounts: budapest01 – budapest30

Passwords: GridBUD01 – GridBUD30

.globus directory contains your private key and certificate.

Passphrase: BUDAPEST

Log to glite-tutor.ct.infn.it computer.



CHARON Directory Contents

\$HOME/CHARON

- system
 - celcore
 - gilda
 - ← core of CHARON
 - ← **activation/deactivation of CHARON**
 - ← hook script for add action of MS
 - ← Module System
 - ← utilities for software deployment to SE
 - migrating
 - modaction
 - module
 - packages
 - software
 - ← common software repository
 - common
- **examples**
 - 01.simple
 - 02.complex
 - 03.parallel
 - 04.autodetection
 - xx.test



Activation of CHARON

Execute script:

`$HOME/CHARON/system/celcore/gilda/migrating/charon-activate`

Activation procedure modifies following files:

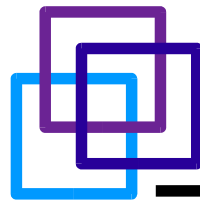
`.bash_profile`

`.bashrc`

It is necessary to open a new terminal session.

Deactivation of CHARON:

`$HOME/CHARON/system/gilda/migrating/charon-deactivate`



Activation of CHARON *continued*

Name of active site



```
*** Welcome to GILDA cluster ***
```

```
=====
You are logged on host : glite-tutor.ct.infn.it
Its architecture is   : i786
```

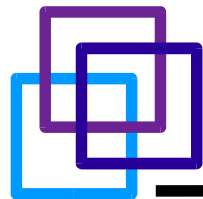
```
-----
Charon Extension Layer (CEL) is enabled.
```

```
If you have any problem with this system you should
contact authors. (More information at WWW portal.)
```

```
***
```

```
http://troll.chemi.muni.cz/whitezone/development/charon
-----
```

pcelinfo – shows above information including basic setup of CEL



Module System

1. list of available applications:

- module
- module avail

2. activation of application:

- module add povray

3. how it works:

- module disp povray

4. list of activated applications:

- module
- module exported*
- module active*

5. configuration of Module System:

- modconfig

***) exported name keeps only module name and version**



Charon System

Virtual organizations

- **gilda** all gilda CEs

Aliases – they define resources more precisely

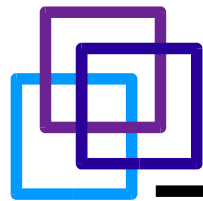
- **short** **CE:** grid010.ct.infn.it:2119/jobmanager-lcgpbs-short
- **work** **CE:** grid004.iucc.ac.il:2119/jobmanager-lcgpbs-short



Examples

\$HOME/CHARON

- **examples**
 - 01.simple
 - `_mytest` ← your work place
 - `input` ← fresh input data
 - `result` ← finished calculation
 - 02.complex
 - 03.parallel
 - 04.autodetection
 - `xx.test`



Simple Job

Scene rendering with povray: `examples/01.simple/_mytest`

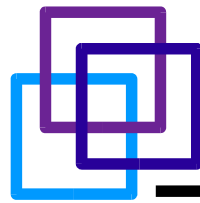
- Contents of job directory

```
laser.pov    render_me*
```

- Job script

```
#!/bin/bash
# activate povray package
module add povray

# render scene
povray -W600 -H600 laser.pov
```



Simple Job *continued*

Job life in CHARON environment

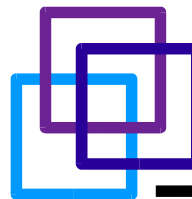
- Job submission
- `$ psubmit short render_me`
- alias* (points to `short`) *job script* (points to `render_me`)

- Job monitoring

```
$ pinfo
```

- Get results

```
$ psync
```



Simple Job *continued*

Information about job (pinfo)

```
Job name      : render_me
Job ID       : https://glite-rb.ct.infn.it:9000/4LNhGMdKn_2oDYKEtkGEJQ
Job title    : render_me (Job type: generic)
Job directory : glite-tutor.ct.infn.it:/home/budapest66/CHARON/examples/01.simple/result
Job project  : -none-
Cluster name : GILDA (Driver: glite)
=====
Alias        : short
Queue       : gilda
Profile     : -none-
-----
NCPU        : 1
Resources   : grid010.ct.infn.it:2119/jobmanager-lcgpbs-short
Properties  : -none-
Sync mode   : gridcopy
-----
Start after : -not defined-
=====
```

+ information about CE/WN and elapsed times

Simple Job *continued*

Contents of Job Directory (finished job)

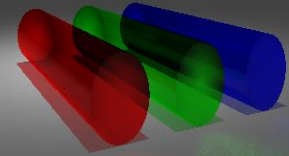
CHARON wrapper script

```
render_me*  
laser.pov  
laser.png  
render_me.stdout  
render_me.jdl  
render_me.ces*  
render_me.cesout  
render_me.info
```

job related data

CHARON related data

laser.png



Complex Job

Analysis of Water Molecules Around LgtC Protein: examples/02.complex/_mytest

- Contents of job directory

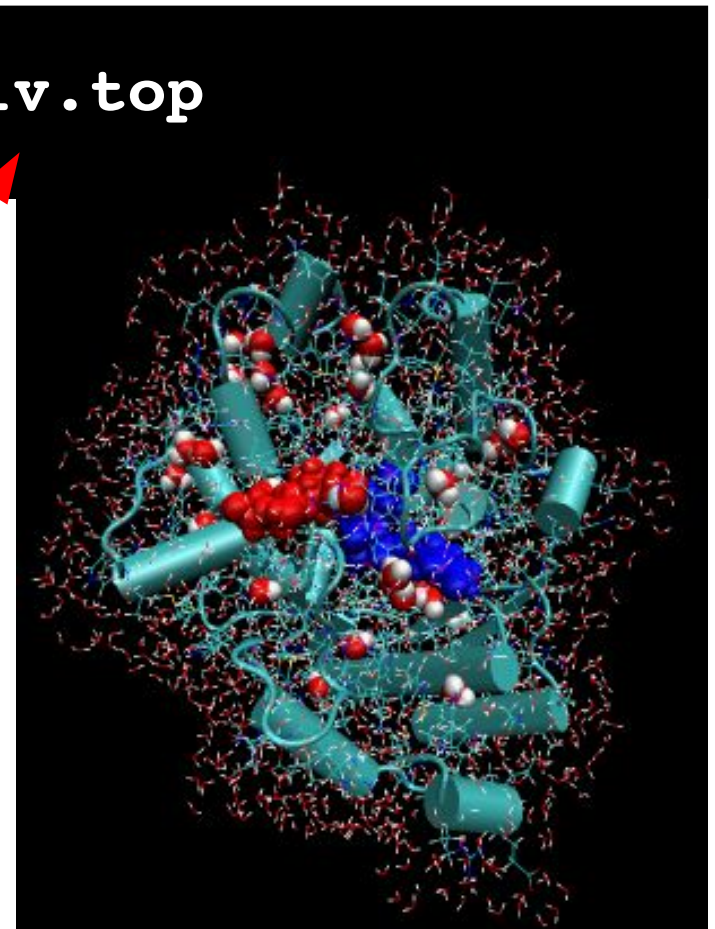
```
get_pdb*  prod050.rst  solv.top
```

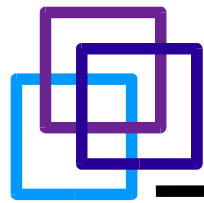
job script

coordinates (AMBER restart file)

topology (AMBER topology file)

The goal is to find tightly bound water molecules and the first solvation shell.





Complex Job *continued*

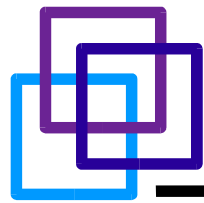
- Job script

```
# load necessary modules
module add cats
module add qhull

# image snapshot
topcrdimage solv.top prod050.rst iprod050.rst

# make rbox file
topcrd2rbox -afp 3.0 solv.top iprod050.rst
iprod050.rbox

# make delaunay triangulation
cat iprod050.rbox | qdelaunay s i T0 output
.....
```



Complex Job *continued*

Job life in CHARON environment

- Job submission

```
$ psubmit short get_pdb
```

alias

job script

- Job monitoring

```
$ pinfo
```

- Get results

```
$ psync
```

Parallel Job

Energy and Gradient Calculation on Cubane Derivative: examples/03.parallel/_mytest

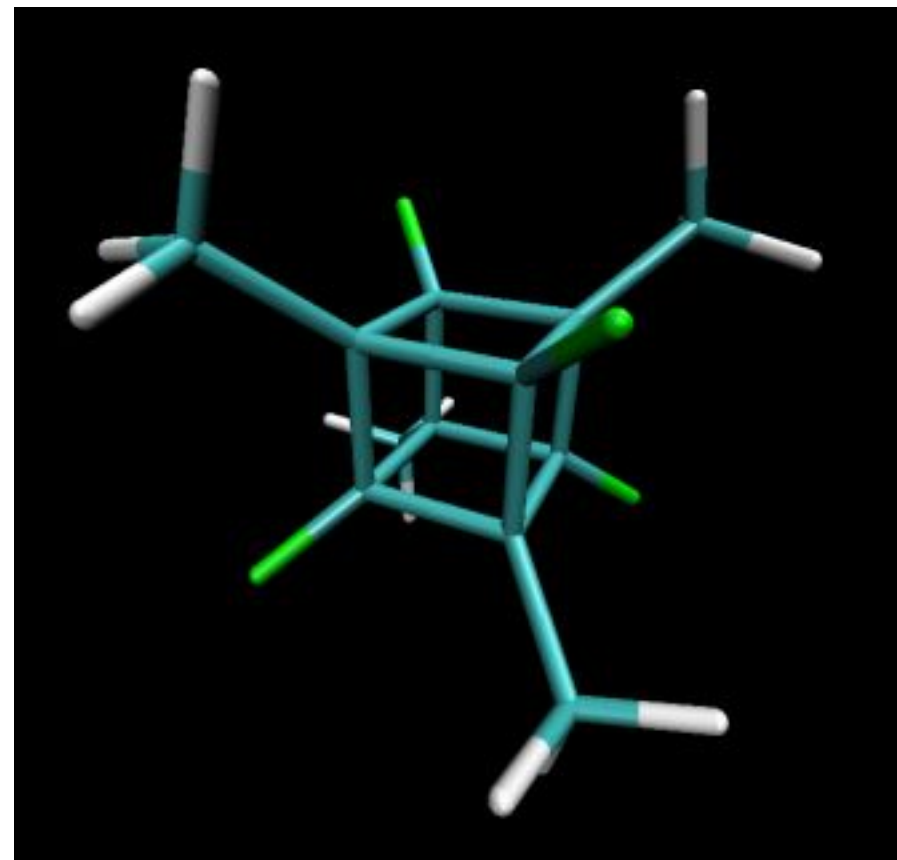
Computational Details

- GAMESS-US
- HF/3-21G - direct SCF

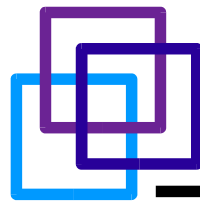
This is not serious calculation!!!!

- pure level of theory
- artificial structure

GAMESS-US is not MPI application.
It uses own parallel engine.
In GILDA, **NCPUs \leq MaxCPUs/node**



artificial cubane derivative



Parallel Job *continued*

- Contents of job directory

```
cubane.inp  run_games*
```

- Job script

```
#!/bin/bash
# activate application
module add games-us

# run games
games cubane > cubane.log
```

Parallel Job *continued*

Job life in CHARON environment

- Job submission – 1 CPU (168 s)

```
$ psubmit short run_gamess
```

- Job submission – 2 CPU (86 s – speedup 1.95x)

```
$ psubmit short run_gamess 2
```

alias

job script

number of CPUs

No changes in job script are required.

Job Autodetection

Povray and gamess-us jobs:

examples/04.autodetection

It is not always necessary to specify job script, in special cases input file can be used too.

- Contents of job directory

```
laser.pov
```

- Job submission

```
$ psubmit short laser.pov
```

alias



povray input file





Discussion

DISCUSSION IS OPEN

Do not forget to show last slide !!!



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