# HP-SEE

## Integrated System for Modeling and data Analysis of complex Biomolecules (ISyMAB)

**www.hp-see.eu**

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HP-SEE
High-Performance Computing Infrastructure for South East Europe's Research Communities



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# ISyMAB

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***Developed by:*** **Dragos Ciobanu-Zabet, Ionut Vasile**
***Scientific collaborations:***

- **Faculty of Physics, University of Bucharest**
- **Faculty of Biology, University of Bucharest**

***Home system (in HP-SEE infrastructure):*** **IFIN_Bio**

***Production systems currently used*:**

- **IFIN_Bio**
- **IFIN_BC**
- **PARADOX**

**Software requirements:**
**NAMD, VMD, OpenGL, VirtualGL, TurboVNC**

# HPC Clusters

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IFIN_Bio

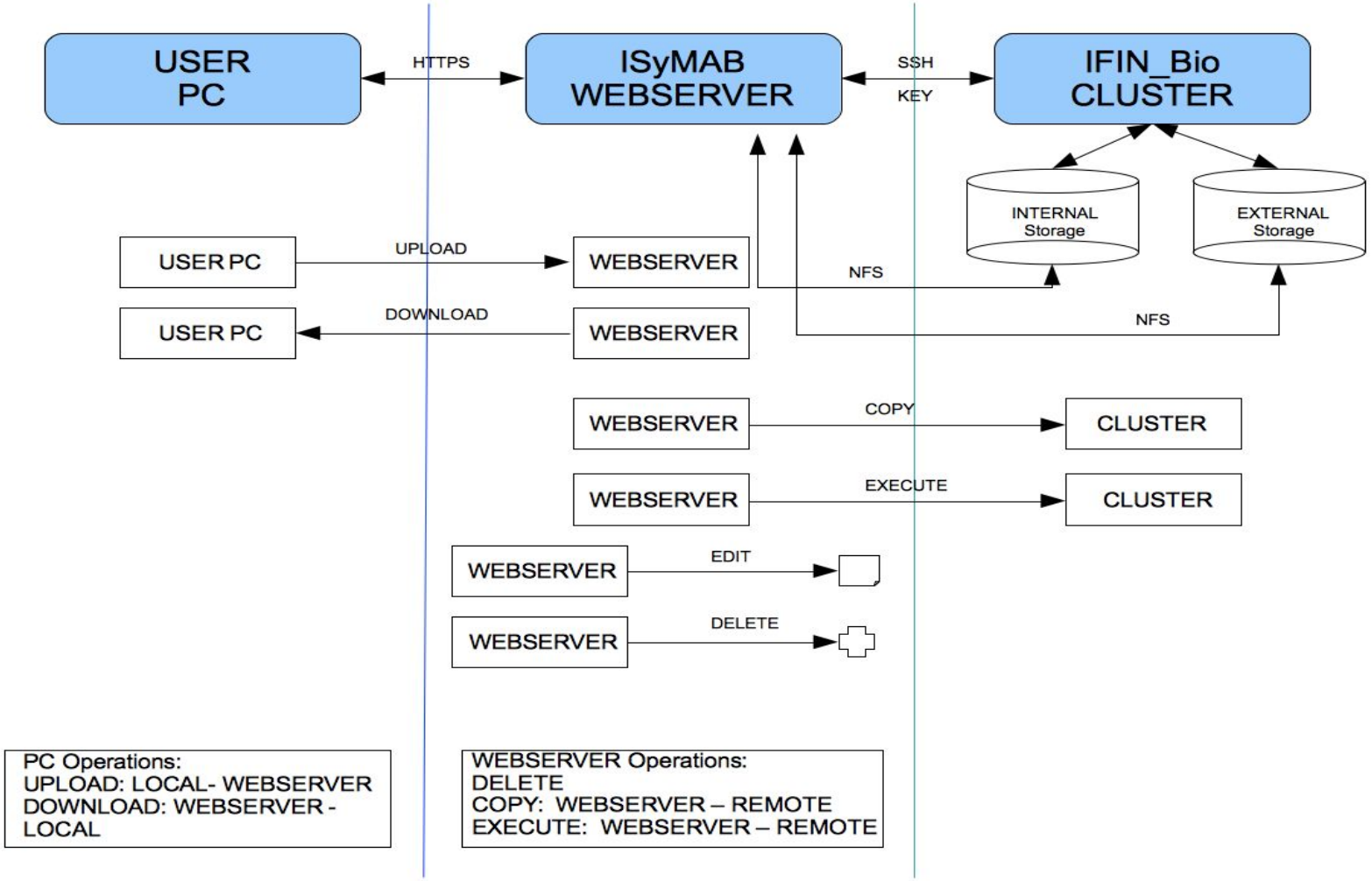
IFIN_BC

PARADOX

http://hpseewiki.ipb.ac.rs/index.php/Resource_centre_IFIN

http://hpseewiki.ipb.ac.rs/index.php/Resource_centre_PARADOX

# App overview



# Login

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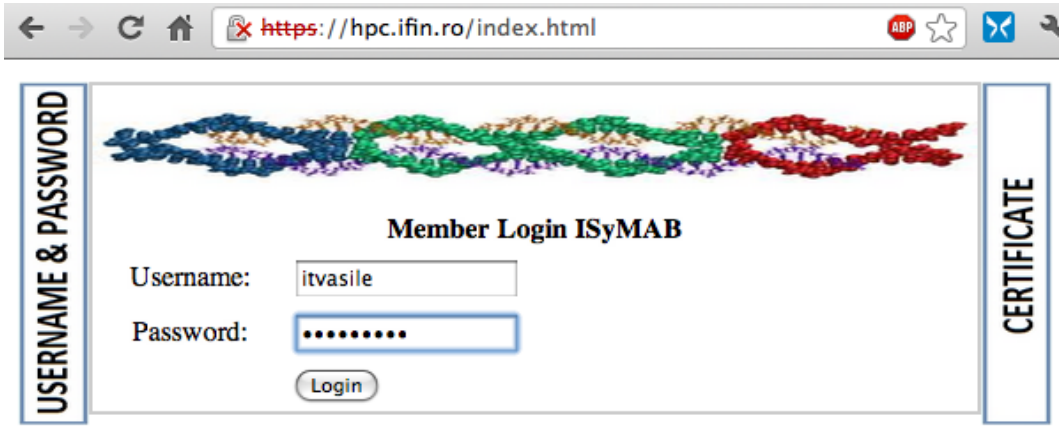



**https://hpc.ifin.ro**

Upon login, the user is checked for access rights on the available production clusters: IFIN_Bio, IFIN_BC and/or PARADOX. Based on this, the user can have further available operations on the cluster(s) on which one have access.

Home

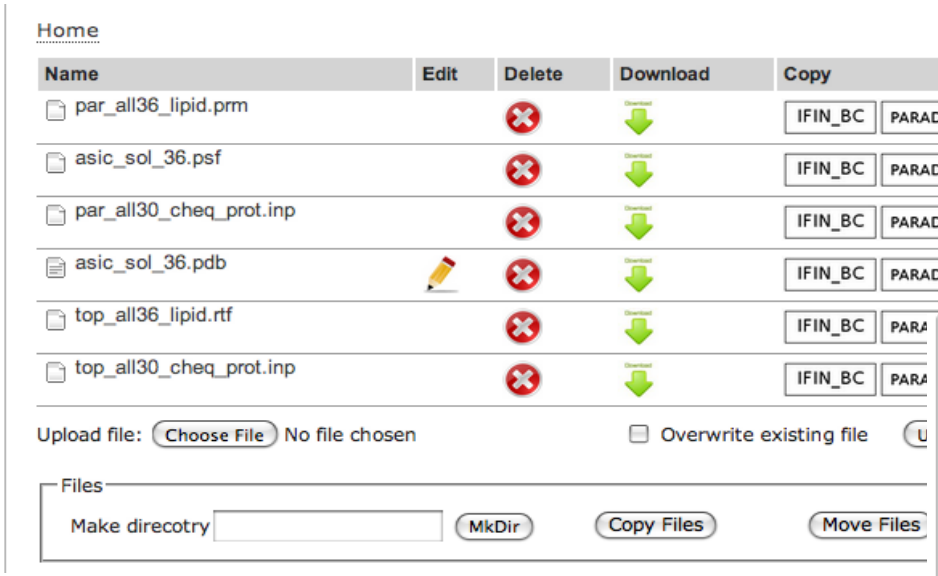
| Name | Edit | Delete | Download | Copy | Execute through PBS | Execute Shell Script | Size |
|---|---|---|---|---|---|---|---|
| HSA | | | - | - | - | - | 0 B |
| asic | | | - | - | - | - | 0 B |
| PDB | | | - | - | - | - | 0 B |
| asic.zip | | | | IFIN_BC PARADOX | - | - | 22.9 Mb |
| itvasile | | | - | - | - | - | 0 B |
| mmtsb | | | - | - | - | - | 0 B |

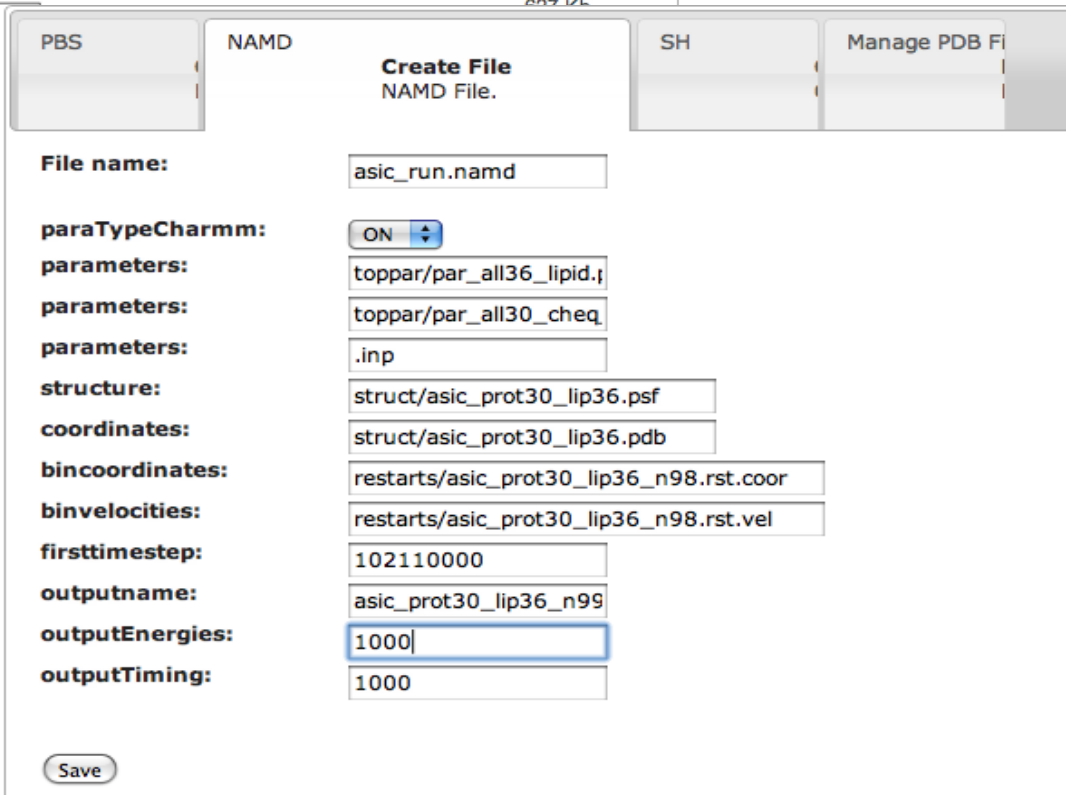
Upload file: Choose File No file chosen  Overwrite existing file  Upload

Opperation Files

Sync files: Sync PARADOX  Sync IFIN_BC

# Some features




- upload archives, pdb, psf, shell scripts, etc.

- create pbs, namd, shell scripts, download pdb from RCSB db.

# Job management module

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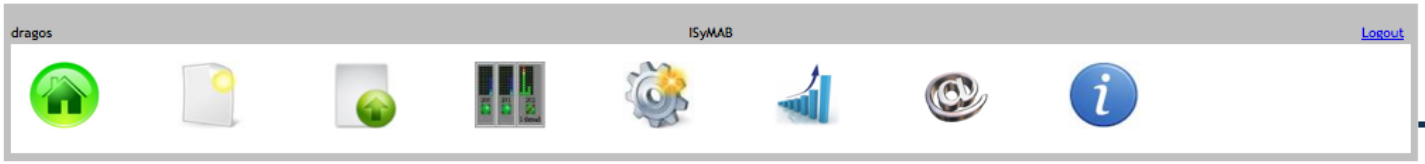


## Torque management system

Queue

**Queue**
Queue Page

| Job ID | Job Name | User | Time Use | Status | Queue | Info | Del Job |
|---|---|---|---|---|---|---|---|
| 1036-247.mdqc01 | mirs-job-247 | oulas | 29:14:18 | R | verylong | Info | Delete |
| 1036-246.mdqc01 | mirs-job-246 | oulas | 42:33:35 | R | verylong | Info | Delete |
| 1036-245.mdqc01 | mirs-job-245 | oulas | 42:43:02 | R | verylong | Info | Delete |
| 1036-244.mdqc01 | mirs-job-244 | oulas | 42:54:23 | R | verylong | Info | Delete |
| 1036-243.mdqc01 | mirs-job-243 | oulas | 31:16:59 | R | verylong | Info | Delete |
| 1036-242.mdqc01 | mirs-job-242 | oulas | 38:24:35 | R | verylong | Info | Delete |
| 1036-241.mdqc01 | mirs-job-241 | oulas | 35:46:00 | R | verylong | Info | Delete |
| 1036-240.mdqc01 | mirs-job-240 | oulas | 42:58:00 | R | verylong | Info | Delete |
| 1036-239.mdqc01 | mirs-job-239 | oulas | 33:31:54 | R | verylong | Info | Delete |
| 1036-238.mdqc01 | mirs-job-238 | oulas | 39:28:17 | R | verylong | Info | Delete |
| 1036-237.mdqc01 | mirs-job-237 | oulas | | | | | |
| 1036-236.mdqc01 | mirs-job-236 | oulas | | | | | |
| 1036-235.mdqc01 | mirs-job-235 | oulas | | | | | |
| 1036-234.mdqc01 | mirs-job-234 | oulas | | | | | |
| 1036-233.mdqc01 | mirs-job-233 | oulas | | | | | |
| 1036-232.mdqc01 | mirs-job-232 | oulas | | | | | |
| 1036-231.mdqc01 | mirs-job-231 | oulas | | | | | |

**verylong**

| | |
|---|---|
| Queue | verylong |
| Queue Type | Execution |
| Priority | 40 |
| State Count | Transit:0 Queued:0 Held:0 Waiting:0 Running:242 Exiting:0 |
| Max Resources | 168:00:00 |
| Default Resources | 168:00:00 |
| Min Resources | 12:00:01 |
| Resources Assigned | -6 |
| Total Jobs | 242 |
| MTime | 1305625051 |
| Max Running | 250 |
| Enabled | True |
| Started | True |
| Route Destinations | |

Close

# Torque

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## PARADOX in Torque job management module: allows the user to see the queue status, server status

PARADOX

| Queue | Max | Tot | Ena | Str | Que | Run | Hld | Wat | Trn | Ext | T |
|---|---|---|---|---|---|---|---|---|---|---|---|
| aginfra | 688 | 0 | yes | yes | 0 | 0 | 0 | 0 | 0 | 0 | E |
| aegis | 688 | 0 | yes | yes | 0 | 0 | 0 | 0 | 0 | 0 | E |
| ops | 5 | 1 | yes | yes | 0 | 1 | 0 | 0 | 0 | 0 | E |
| cms | 688 | 0 | yes | yes | 0 | 0 | 0 | 0 | 0 | 0 | E |
| seegrid | 688 | 26 | yes | yes | 0 | 26 | 0 | 0 | 0 | 0 | E |
| desktopg | 30 | 48 | yes | yes | 18 | 30 | 0 | 0 | 0 | 0 | E |
| see | 688 | 9 | yes | yes | 0 | 6 | 0 | 3 | 0 | 0 | E |
| sgdemo | 0 | 0 | yes | yes | 0 | 0 | 0 | 0 | 0 | 0 | E |
| atlas | 688 | 0 | yes | yes | 0 | 0 | 0 | 0 | 0 | 0 | E |
| hpsee | 688 | 481 | yes | yes | 453 | 28 | 0 | 0 | 0 | 0 | E |
| dteam | 5 | 0 | yes | yes | 0 | 0 | 0 | 0 | 0 | 0 | E |

| Server | Max | Tot | Que | Run | Hld | Wat | Trn | Ext | Status |
|---|---|---|---|---|---|---|---|---|---|
| ce64.ipb.ac.rs | 0 | 564 | 471 | 90 | 0 | 3 | 0 | 0 | Active |

# ISyMAB MMTSB

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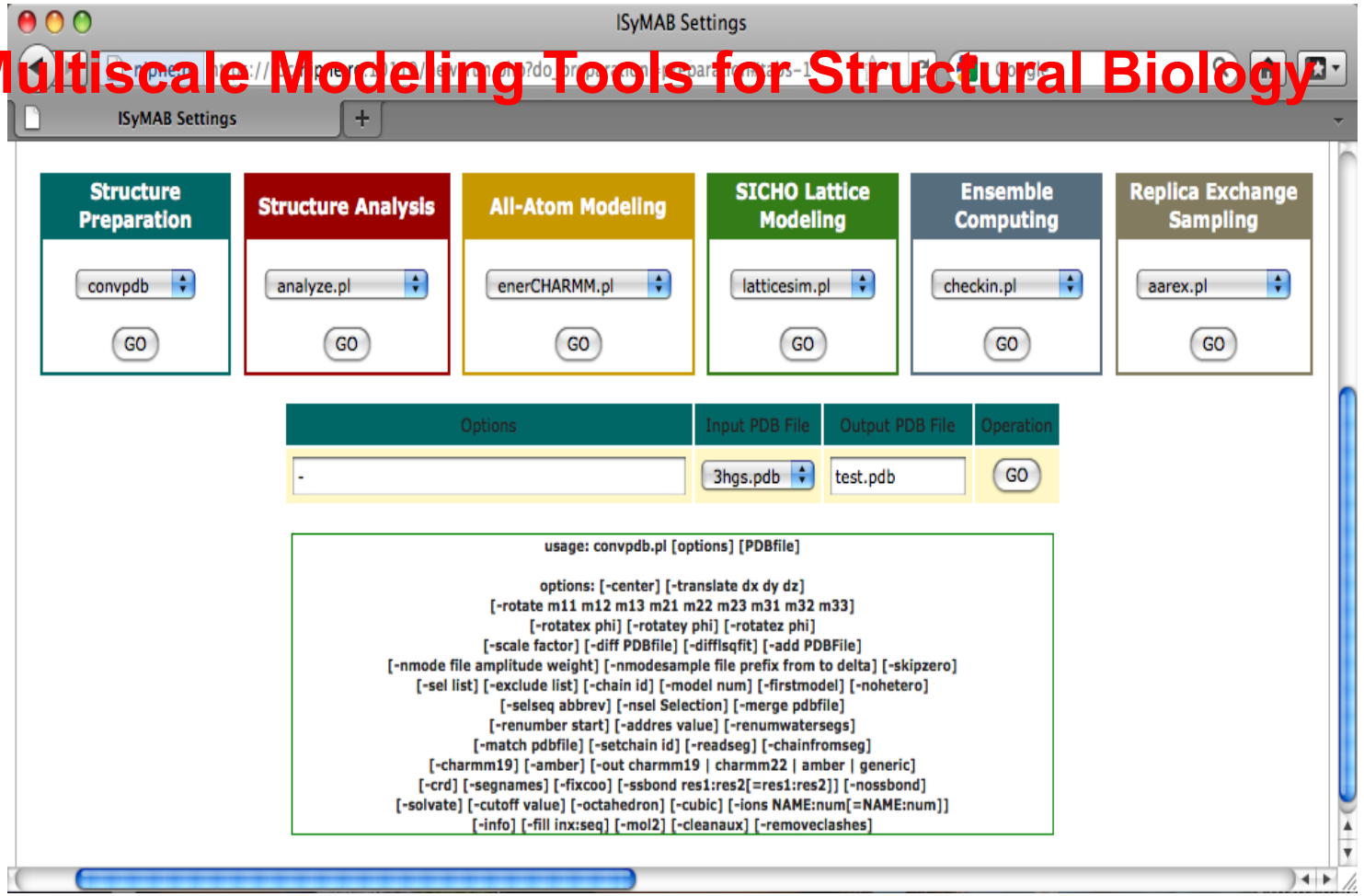
## Multiscale Modeling Tools for Structural Biology




You can select a function from the drop-down menus and push “GO”. Then enter parameters, respecting the syntax mentioned and the output file and “GO”.

# ISyMAB MMTSB

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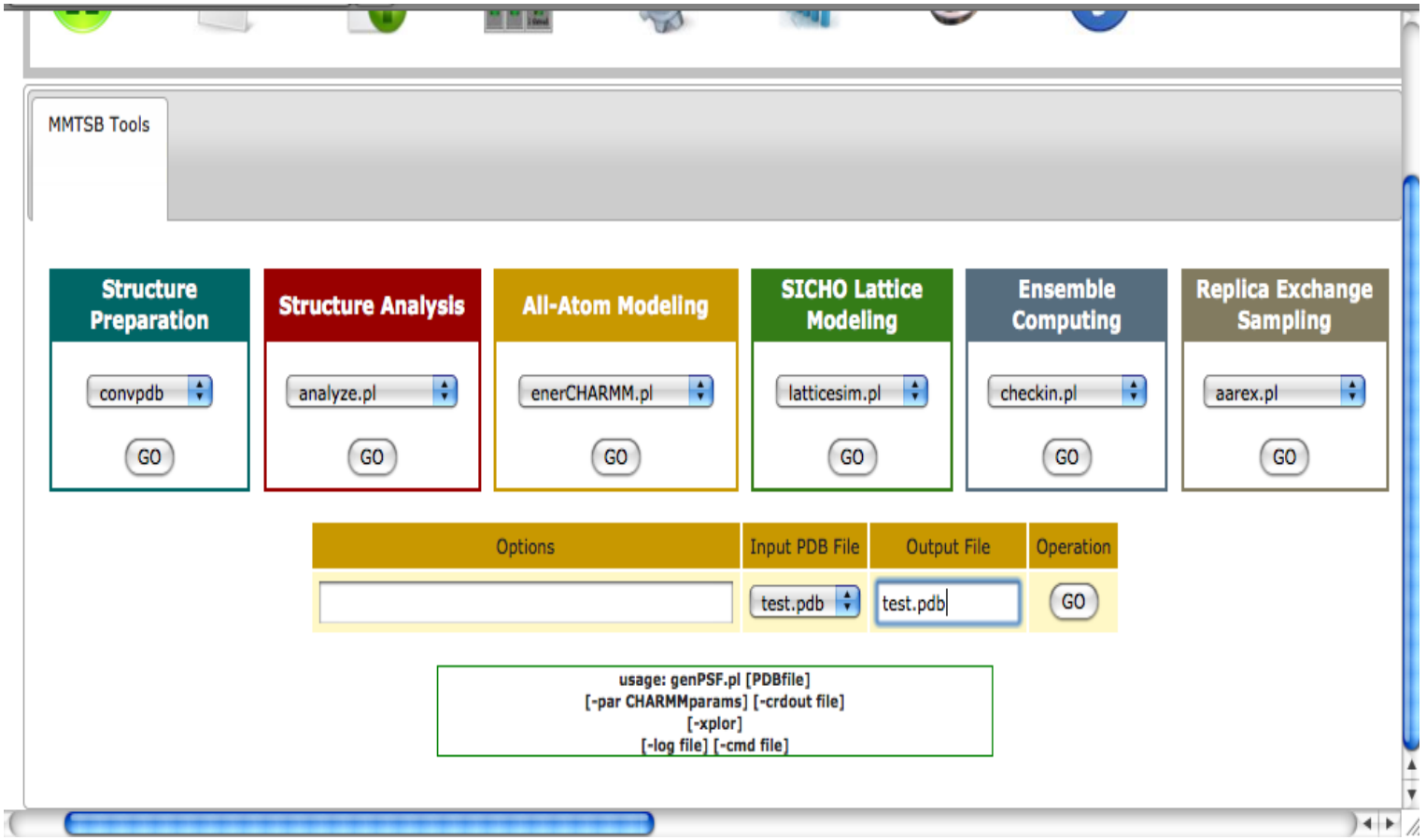
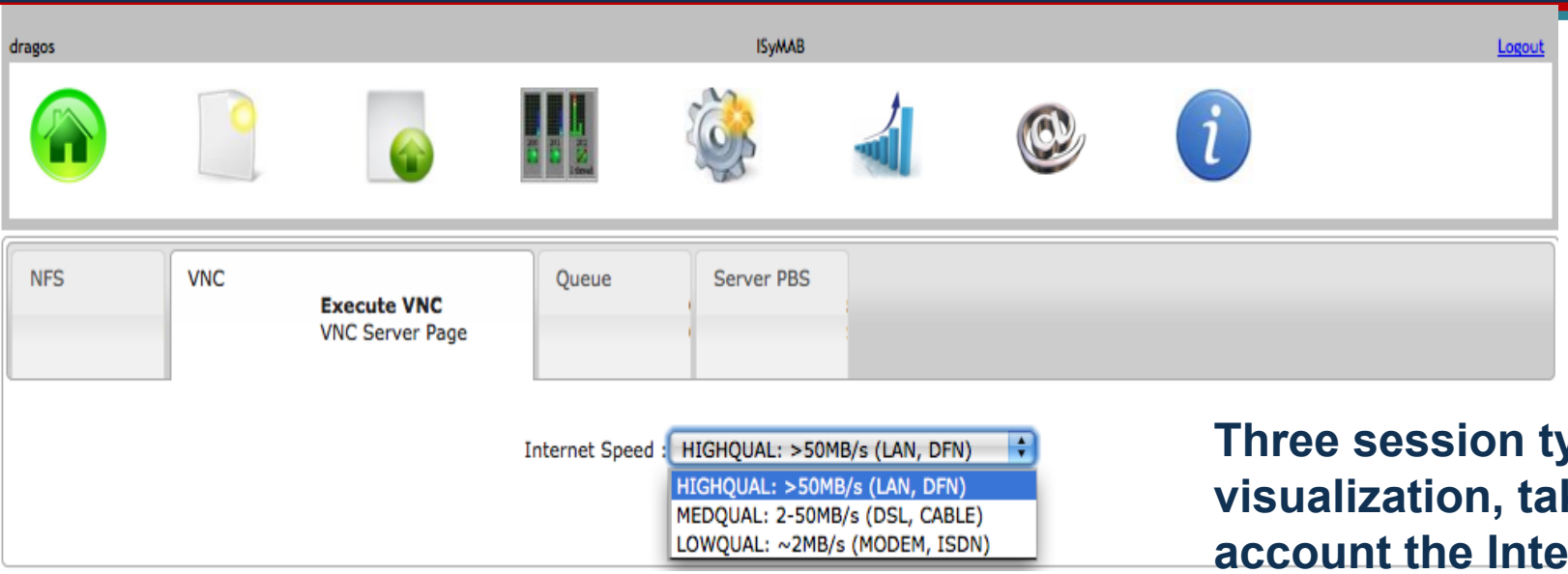
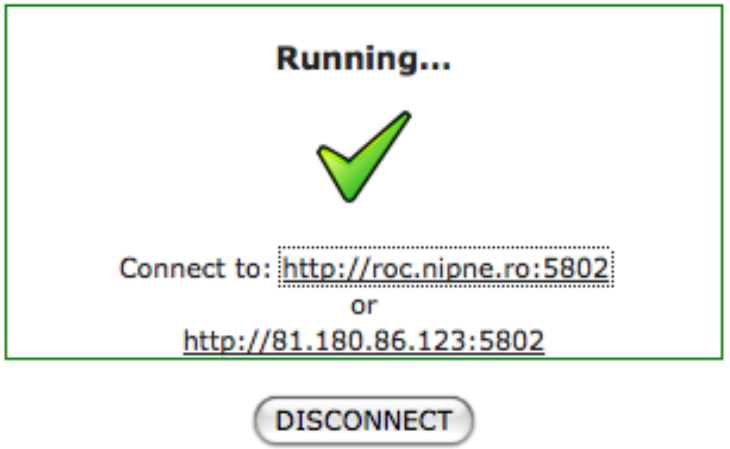



**The functions are sorted in 6 color-coded groups for easy usage.**

**The output files can then be found in the working directory, using the integrated file manager.**

# ISyMAB remote visualization

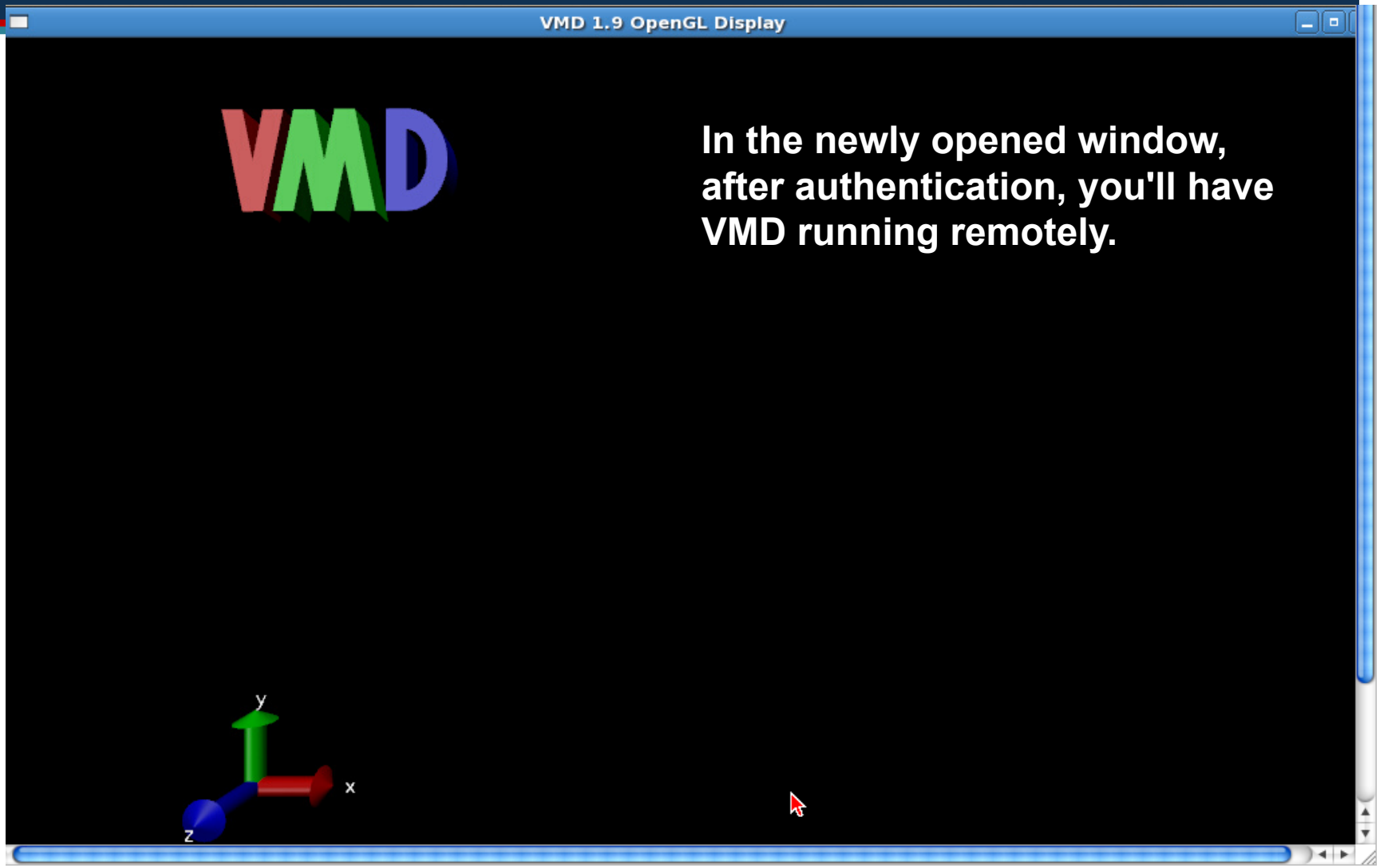



**Three session types for remote visualization, taking into the account the Internet speed at which you can connect to the server.**

**Upon selection, you click GO and it will be opened a new window to the Analysis server. In this page you will have the possibility to end the session hitting "Disconnect".**

# ISyMAB remote visualization

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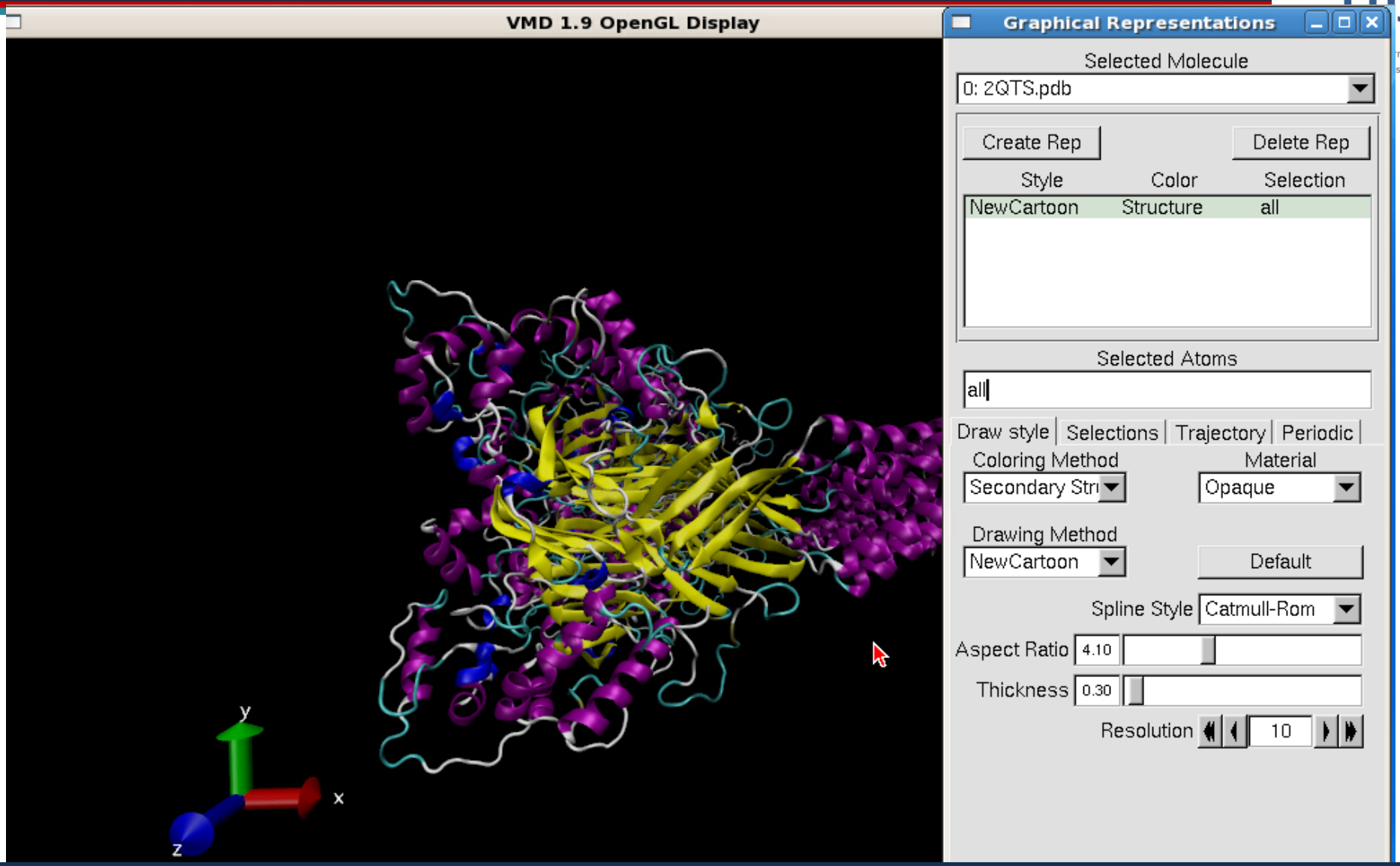
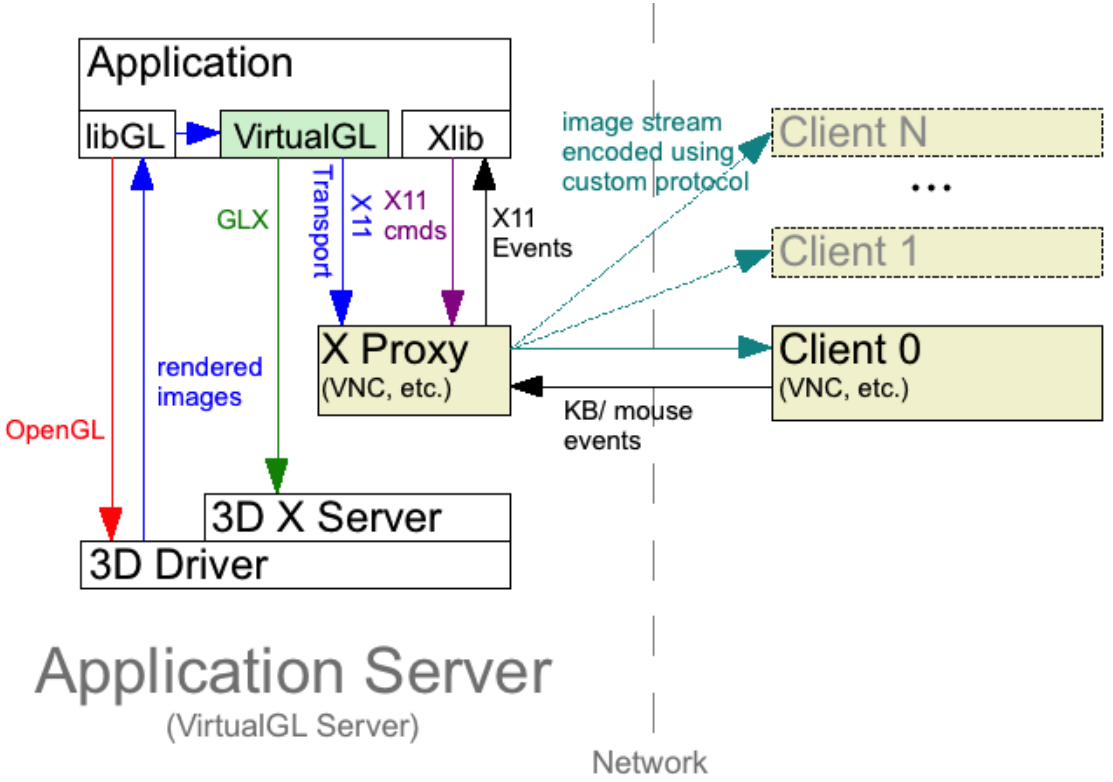
# ISyMAB remote visualization



# ISyMAB remote visualization




**VMD with OpenGL support**
**TurboVNC with VirtualGL open source packages => remote OpenGL apps with 3D hardware support**

**All of this because we don't have acces to the 3D driver of the remote graphic card**

# Benchmark

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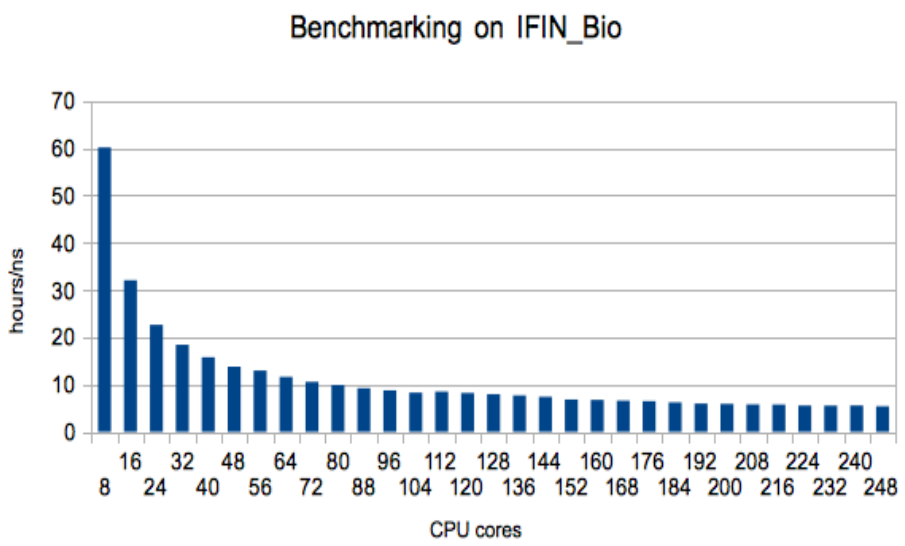
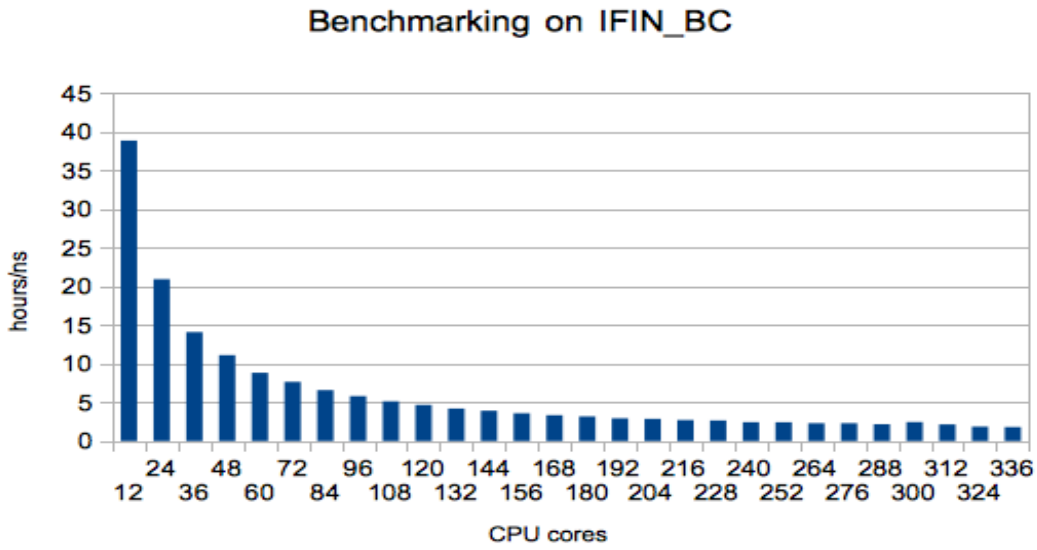
## Benchmarking:

**The benchmarks were performed on IFIN_Bio (left side) and IFIN_BC (right side):**
**- ApoA1 (92,224 atoms, 12A cutoff + PME every 4 steps, periodic)**





## Final words and perspectives

- after porting to PARADOX we had to retest the application and some code needed to be rewritten, other parts needed improvements
- based on user rights, we could give access to other softwares which are not free: CHARMM, AMBER...
- the entire interface needs simplification

# Thank You!