

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

**HP-SEE**  
[www.hp-see.eu](http://www.hp-see.eu)



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**HP-SEE**

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





***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_IFIN)

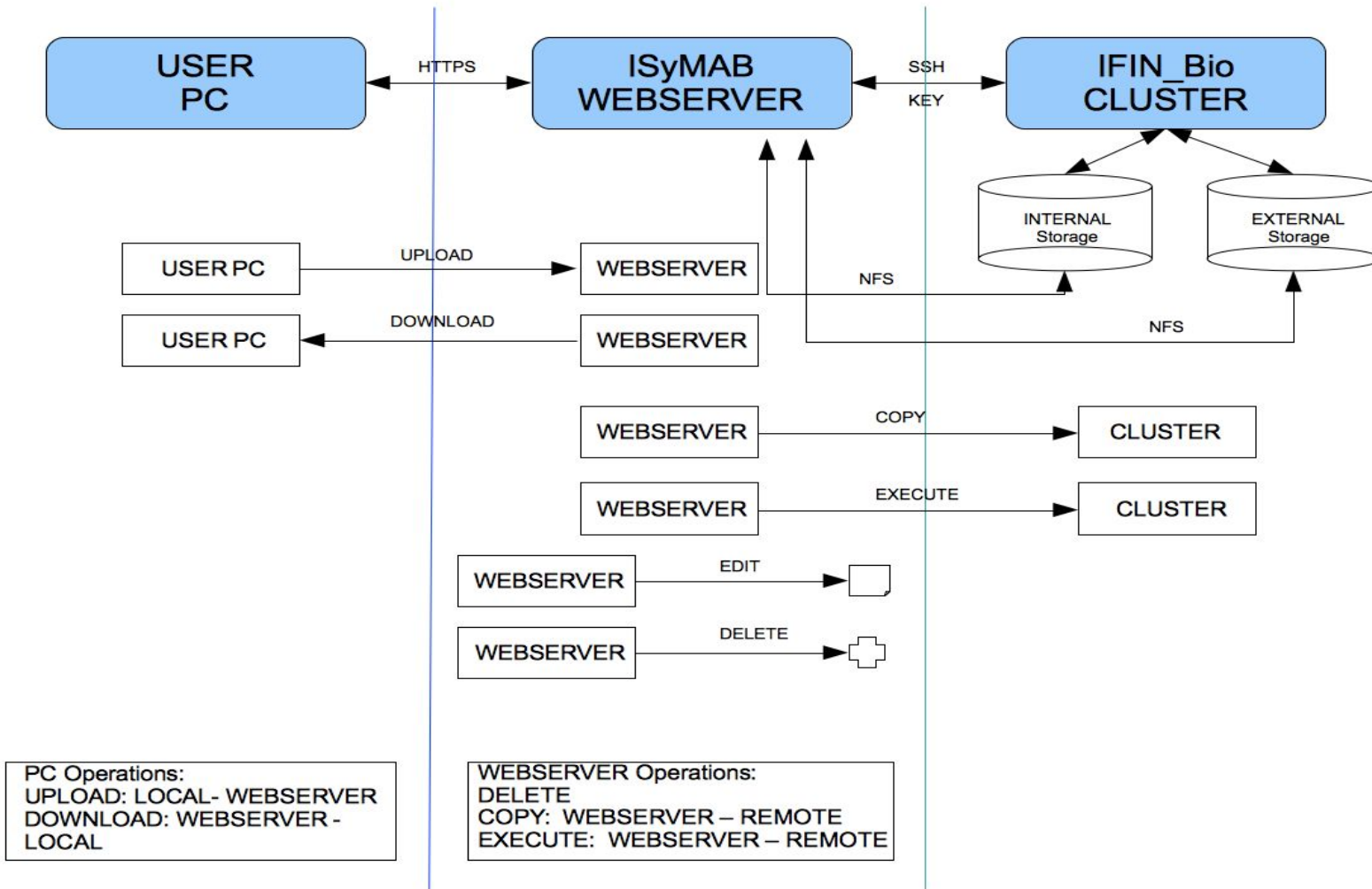
[http://hpseewiki.ipb.ac.rs/index.php/Resource\\_centre\\_PARADOX](http://hpseewiki.ipb.ac.rs/index.php/Resource_centre_PARADOX)

# App overview



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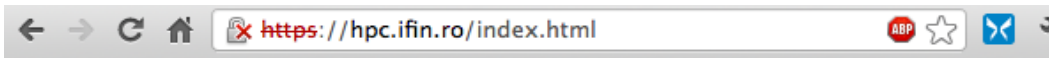


# Login



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**Member Login ISyMAB**

Username:

Password:

**USERNAME & PASSWORD** (left vertical label)

**CERTIFICATE** (right vertical label)

<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				<input type="button" value="IFIN_BC"/> <input type="button" value="PARADOX"/>	-	-	22.9 Mb
itvasile			-	-	-	-	0 B
mmtsb			-	-	-	-	0 B

Upload file:  No file chosen

Overwrite existing file

Sync files:

# Some features



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Home

Name	Edit	Delete	Download	Copy	Execute through PBS	Execute Shell Script	Size
par_all36_lipid.prm				IFIN_BC PARADOX	-	-	26.5 Kb
asic_sol_36.psf				IFIN_BC PARADOX	-	-	141.1 Mb
par_all30_cheq_prot.inp				IFIN_BC PARADOX	-	-	137.9 Kb
asic_sol_36.pdb				IFIN_BC PARADOX	IFIN_BC PARADOX	IFIN_BC PARADOX	58 Mb
top_all36_lipid.rtf				IFIN_BC PARADOX			607 Kb
top_all30_cheq_prot.inp				IFIN_BC PARADOX			

Upload file:  No file chosen

Overwrite existing file

Files

Make directory

PBS NAMD SH Manage PDB File

**Create File**  
NAMD File.

**File name:**

**paraTypeCharmm:**

**parameters:**

**parameters:**

**parameters:**

**structure:**

**coordinates:**

**bincoordinates:**

**binvelocities:**

**firsttimestep:**

**outputname:**

**outputEnergies:**

**outputTiming:**

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

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

# Job management module



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dragos ISyMAB [Logout](#)

## Torque management system

Queue **Queue Page**

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



### 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





## Multiscale Modeling Tools for Structural Biology

ISyMAB Settings

Structure Preparation: convpdb

Structure Analysis: analyze.pl

All-Atom Modeling: enerCHARMM.pl

SICH0 Lattice Modeling: latticesim.pl

Ensemble Computing: checkin.pl

Replica Exchange Sampling: aarex.pl

Options	Input PDB File	Output PDB File	Operation
-	3hgs.pdb	test.pdb	GO

```

usage: convpdb.pl [options] [PDBfile]

options: [-center] [-translate dx dy dz]
[-rotate m11 m12 m13 m21 m22 m23 m31 m32 m33]
[-rotatex phi] [-rotatey phi] [-rotatez phi]
[-scale factor] [-diff PDBfile] [-diffsqfit] [-add PDBFile]
[-nmode file amplitude weight] [-nmodesample file prefix from to delta] [-skipzero]
[-sel list] [-exclude list] [-chain id] [-model num] [-firstmodel] [-nohetero]
[-selseq abbrev] [-nset Selection] [-merge pdbfile]
[-renumber start] [-address value] [-renumwatersegs]
[-match pdbfile] [-setchain id] [-readseg] [-chainfromseg]
[-charmm19] [-amber] [-out charmm19 | charmm22 | amber | generic]
[-crd] [-segnames] [-fixcoo] [-ssbond res1:res2[=res1:res2]] [-nossbond]
[-solvate] [-cutoff value] [-octahedron] [-cubic] [-ions NAME:num[=NAME:num]]
[-info] [-fill inx:seq] [-mol2] [-cleanaux] [-removeclashes]
    
```

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”.



MMTSB Tools

Structure Preparation	Structure Analysis	All-Atom Modeling	SICHO Lattice Modeling	Ensemble Computing	Replica Exchange Sampling
convpdb	analyze.pl	enerCHARMM.pl	latticesim.pl	checkin.pl	aarex.pl
GO	GO	GO	GO	GO	GO

Options	Input PDB File	Output File	Operation
	test.pdb	test.pdb	GO

```
usage: genPSF.pl [PDBfile]
       [-par CHARMMparams] [-crdout file]
       [-xplor]
       [-log file] [-cmd file]
```

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



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dragos ISyMAB Logout

NFS VNC **Execute VNC** Queue Server PBS  
VNC Server Page

Internet Speed: HIGHQUAL: >50MB/s (LAN, DFN)  
HIGHQUAL: >50MB/s (LAN, DFN)  
MEDQUAL: 2-50MB/s (DSL, CABLE)  
LOWQUAL: ~2MB/s (MODEM, ISDN)

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

**Running...**

Connect to: <http://roc.nipne.ro:5802>  
or  
<http://81.180.86.123:5802>

DISCONNECT

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



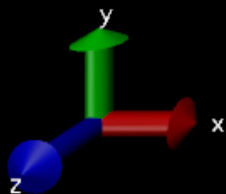
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VMD 1.9 OpenGL Display

**VMD**

In the newly opened window,  
after authentication, you'll have  
VMD running remotely.



# ISyMAB remote visualization



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VMD 1.9 OpenGL Display

Graphical Representations

Selected Molecule

0: 2QTS.pdb

Create Rep

Delete Rep

Style	Color	Selection
NewCartoon	Structure	all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method  
Secondary Stri

Material  
Opaque

Drawing Method  
NewCartoon

Default

Spline Style  
Catmull-Rom

Aspect Ratio 4.10

Thickness 0.30

Resolution 10

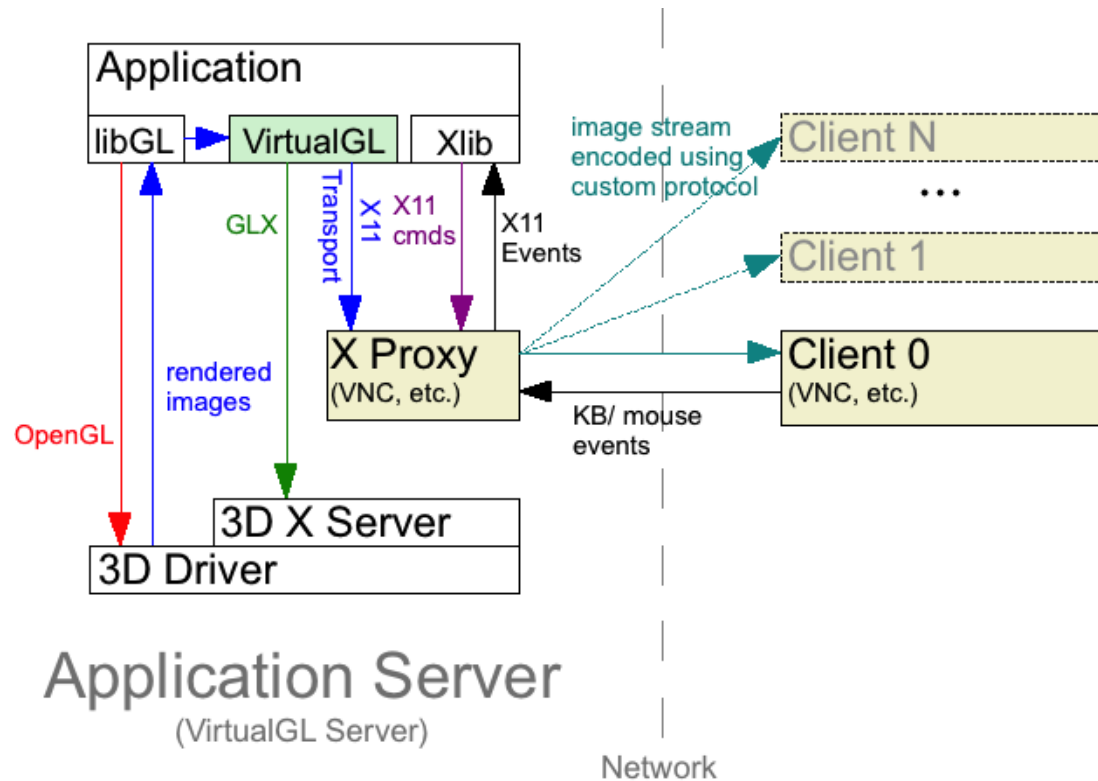


# ISyMAB remote visualization



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VMD with OpenGL support

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

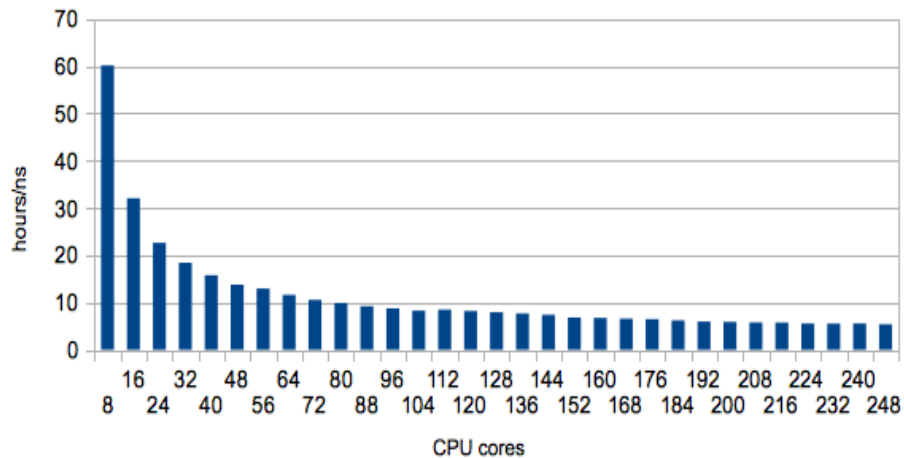
All of this because we don't have access to the 3D driver of the remote graphic card



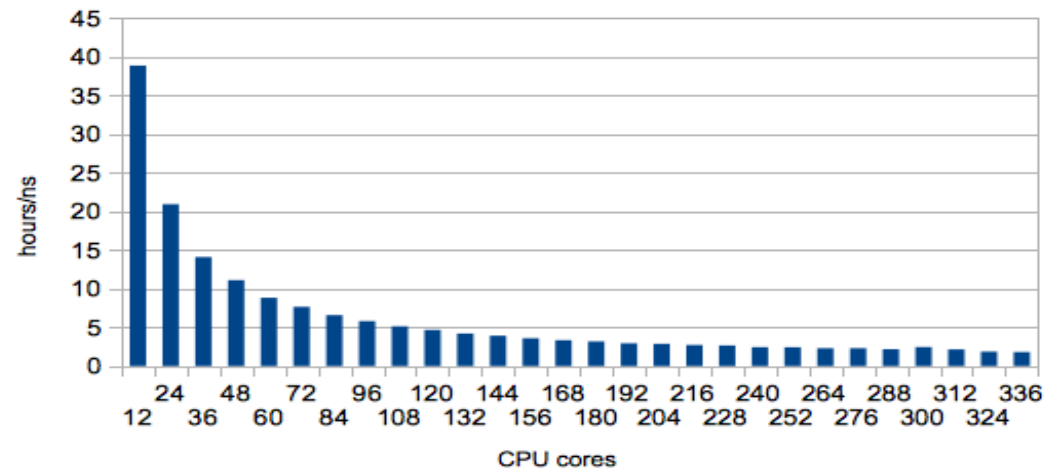
### Benchmarking:

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)

Benchmarking on IFIN\_Bio



Benchmarking on IFIN\_BC





## 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!