

Software tools for HPC users at IFIN-HH

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IFIN-HH

Outline:

- current HPC infrastructure**
- network services**
- available software tools**
- ISyMAB**

HPC infrastructure



IFIN_Bio Cluster

Myrinet 2000
2x Quad-core Xeon

HPC infrastructure



IFIN_BC Cluster

Blades
Infiniband 4X
2x Quad-core Opteron
2x PowerXCell 8i
2x Hex-Core Xeon

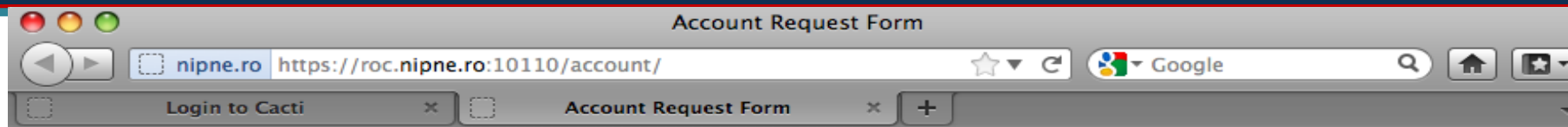


30-11-2011

HPC infrastructure specs

Feature	IFIN_Bio	IFIN_BC		
Server name	Dell PowerEdge 1950 III	IBM QS22	IBM LS22	IBM HS22
Processor	Intel Xeon E5430 (Quad-Core)	IBM PowerXCell 8i	AMD Opteron 2376 HE	Intel Xeon X5650
Clock frequency (f)	2.66 GHz	3.2 GHz	2.3GHz	2.67GHz
Cores per CPU	4	1xPPE + 8xSPE	4	6
CPUs per node	2	2	2	2
FSB	1333 MHz	1066 MHz	1000 MHz	3200 MHz
2-level cash memory per CPU	12 MB	512 KB	512 KB	6 x 256 KB
RAM on node	16 GB (8x2GB DDR2 ECC)	32 GB	8GB	24 GB
Nodes within cluster	32	16	10	28
Overall number of CPUs	64	32 PowerXCell	20	56
Overall number of cores (n)	256	32xPPE + 256xSPE	80	336
Overall RAM	512 GB	512 GB	80GB	672 GB
Harddisk per node	500 GB (SATA II)	8GB Modular Flash Drive (SSD)	76GB; 146GB (SAS)	500GB (SAS)
Network (fastest)	1x Myrinet 2000 2Gbps	Infiniband 4X DDR 20 Gbps	Infiniband 4X DDR 20 Gbps	Infiniband 4X
MPI flavour	ch_mx 1.2.7	OpenMPI 1.3.2	OpenMPI 1.3.2	OpenMPI 1.4.3
Operating System	CentOS 5.4	Fedora 9	CentOS 5.4	Scientific Linux 5.7
Flops per tact (k)	4	4	4	4

HPC Account Request



An account request form has been implemented in order to ease the interaction with new users.

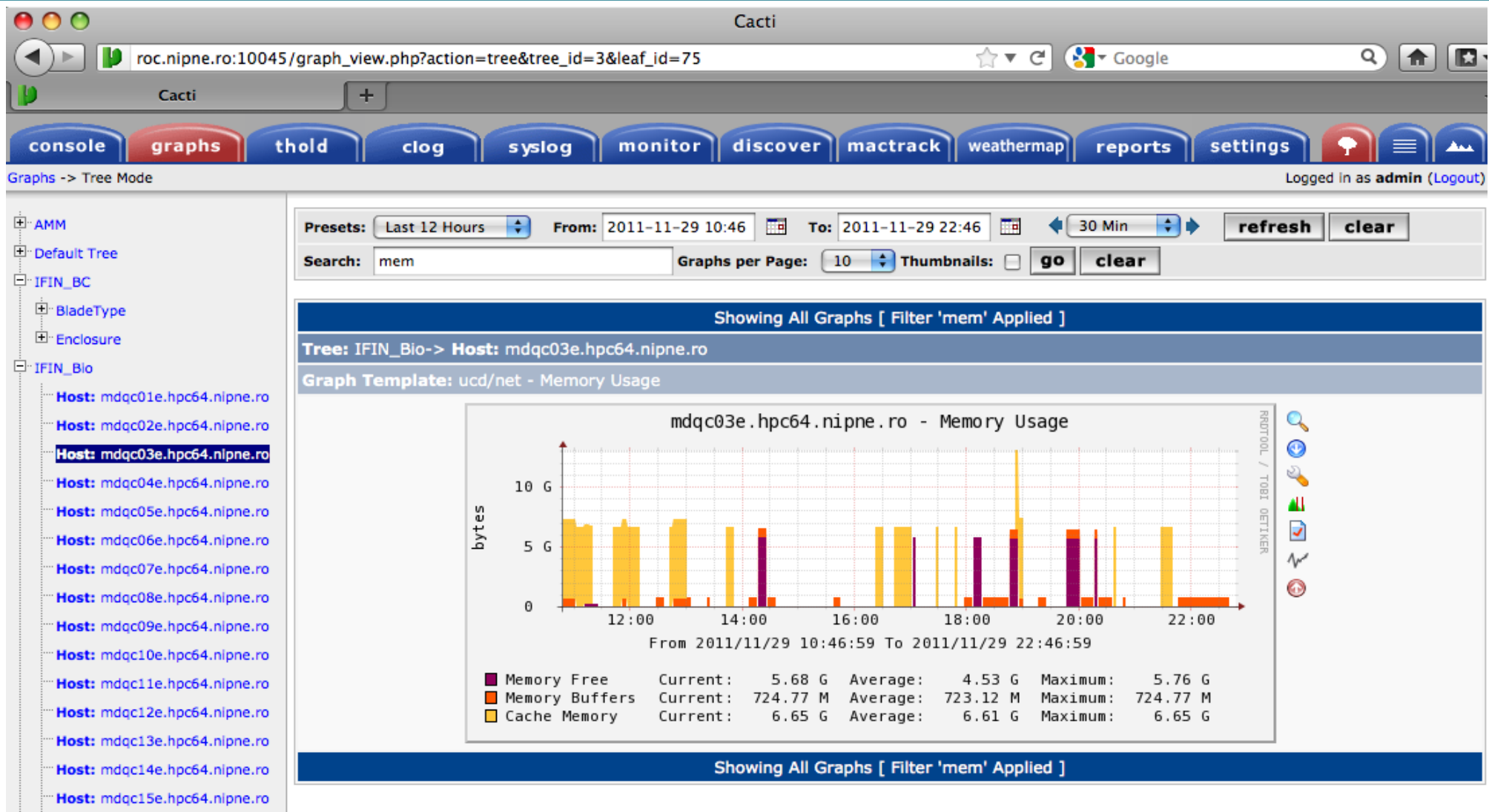
Account Request

HP-SEE Account Request Form

Requested username:	<input type="text"/>
First Name:	<input type="text"/>
Last Name:	<input type="text"/>
Organization:	<input type="text"/>
Address:	<input type="text"/>
Phone:	<input type="text"/>
E-mail:	<input type="text"/>
Project Name:	<input type="text"/>
Description of work to be done:	<input type="text"/>
Choose cluster:	<input type="text" value="Cluster IFIN_BIO"/>
Type verification image:	<input type="text"/> * 1161

Submit

Cluster monitoring: Cacti



Available software tools

Open-source scientific software packages:

NAMD
VMD
MMTSB

Commercial scientific softwares:

CHARMM
Gaussian
VASP
Turbomole
Matlab

Generic softwares:

charm++
GotoBLAS
FFTW
MPI: MPICH-MX, OpenMPI, MVAPICH
GNU Toolchain, OpenMP
Ssh
Torque
IBM Software Kit for Multicore Acceleration
TotalView

In-house developed:

ISyMAB

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

www.hp-see.eu



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for South East Europe's Research Communities

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



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Short description

We aim at providing an efficient tool for data analysis in the framework of the simulation and modeling of large biomolecular systems by means of parallel molecular dynamics codes designed for high-performance computing (NAMD). The main focus is in the modeling of the G Protein-Coupled Receptors, which are found in a wide range of species, and are involved in signalling from the outside to the inside of the cells.

The application builds a remote access framework on NAMD clusters which offers the users an integrated interface with analysis tools, which will make possible fast data analysis of complex simulation outputs directly on the remote systems. The users provide the initial parameters of the MD simulation, launch jobs, and make various data analysis on the output files.

- ❑ Developers: IFIN-HH/DPETI, Romania**

ISyMAB: progress of the work



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ISyMAB is currently in beta stage, developed and hosted on IFIN_Bio, which is part of the HP-SEE infrastructure. At this stage, it does not need porting to another site.

Results obtained according to the planning from D4.1 (see next images):

- redesign and improvement of the web interface
- implementation of the torque (PBS) job management system within web interface: procedures to submit and manage the simulation jobs
- access the network shared folders within the cluster: local storage (Myrinet 2G interconnection) and permanent storage (Gigabit Ethernet interconnection).

ISyMAB: progress of the work



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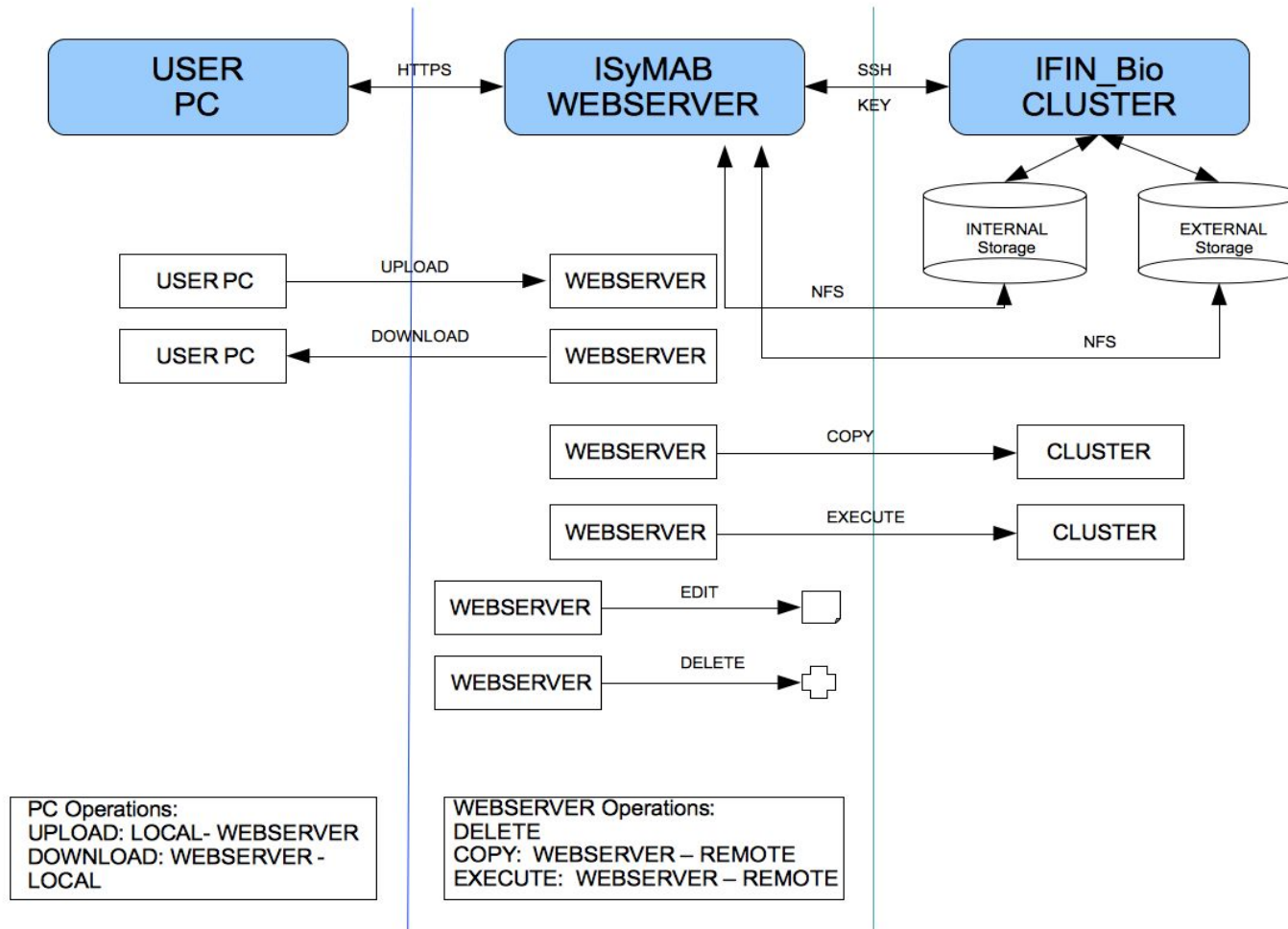
- development of the module which features the **MMTSB (Multiscale Modeling Tools for Structural Biology)** toolset
- integrate a function for downloading PDB files directly from the Protein data bank (<http://www.rcsb.org>)
- integrate the VirtualGL open source package, which has the ability to run OpenGL applications (in our case VMD) with full 3D hardware acceleration, in conjunction with TurboVNC (for remote visualization)
- development of a management module which controls dynamically the allocation of sessions for remote visualization

ISyMAB overview scheme(1)



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ISyMAB login page (2)



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ISyMAB Login

nipne.ro https://roc.nipne.ro:10110/new/index.html

ISyMAB Login

Reachable from the Internet,
but restricted to developers and
some testers.

USERNAME & PASSWORD

Member Login ISyMAB

Username:

Password:

Login

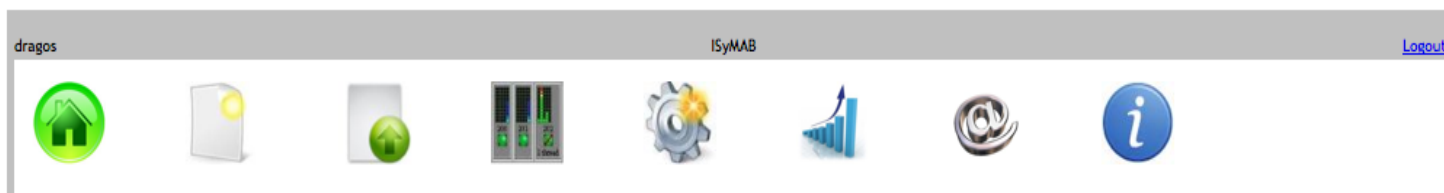
CERTIFICATE

ISyMAB templates for files (3)



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File name:

paraTypeCharm:

ON

parameters:

par_all27_lipid.inp

parameters:

par_all22_prot.inp

parameters:

par_ret_chloride.inp

structure:

sr-chaina_mb_new3_xplor.psf

coordinates:

sr-chaina_mb_new3.pdb

bincoordinates:

sr-chaina_mb_new3_n26.rst.coor

binvelocities:

sr-chaina_mb_new3_n26.rst.vel

firsttimestep:

30110000

outputname:

sr2_n27.out

outputEnergies:

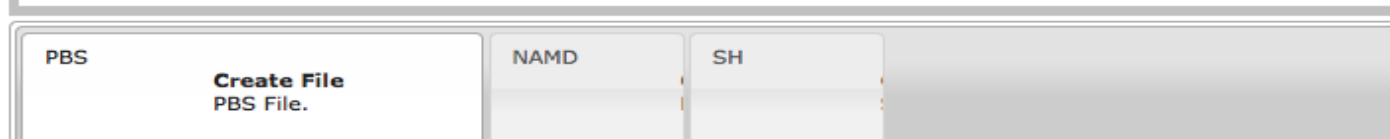
1000

outputTiming:

1000

Send to File

NAMD input file



File name:

Job name:

wtNAMD-x86_64_mpi

Node number:

32

1 - 32 nodes

Core Number:

8

1 - 8 cores

Queue to submit:

long => cputime 12h

Input file:

sr2_n27

Output file:

sr2_n27

Com Proto:

SSH

Email:

admin@nipne.ro

Report:

Abort ☐ Begin ☐ End ☐ None ☒

Send File

PBS job
description file

IsyMAB file management (4)



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Local ISyMAB WebServer Permanent Internal

Home

Name	Edit	Delete	Download	Copy	Execute	Size
test.sh						8 B
pbs.sh						1.7 Kb
shell.sh						1.7 Kb

Upload file: Browse... ☐ Overwrite existing file Upload

ISyMAB Logout

Permanent Storage (Remote) Internal

Home

Name	Edit	Delete	Download	Copy	Execute	Size
lost+found	-		-	-	-	0 B
HG 585.pdf	-				-	1.4 Mb
K1.mdqc19.hpc64.nipne.ro	-				-	1.5 Gb
K1.mdqc20.hpc64.nipne.ro	-				-	1.4 Gb
2011-04-19 10.55.37.jpg	-				-	1.4 Mb

Upload file: Browse... ☐ Overwrite existing file Upload

Manage files located locally on the webserver, on the Permanent Storage or on the Internal Cluster Storage; here you can Edit, Delete, Download, Upload, Copy, or send the file to Execute on the cluster

ISyMAB job management (5)



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Queue Queue Queue Page Server PBS

Queue	Max	Tot	Ena	Str	Que	Run	Hld	Wat	Trn	Ext	T	Details	Info
hpc_med	10	0	yes	yes	0	0	0	0	0	0	E	Detail	Info
small	50	0	yes	yes	0	0	0	0	0	0	E	Detail	Info
default	300	0	yes	yes	0	0	0	0	0	0	R	Detail	Info
medium	50	0	yes	yes	0	0	0	0	0	0	E	Detail	Info
long	50	0	yes	yes	0	0	0	0	0	0	E	Detail	Info
hpc_all	2	0	yes	yes	0	0	0	0	0	0	E	Detail	Info
verylong	250	242	yes	yes	0	242	0	0	0	0	E	Detail	Info

you can check the general informations for each PBS server and the queues defined on it

ISyMAB Logout

Queue Server PBS

Server PBS Server PBS Page

Server	Max	Tot	Que	Run	Hld	Wat	Trn	Ext	Status	Info
mdqc01.hpc64.nip	0	242	0	242	0	0	0	0	Active	Info

mdqc01.hpc64.nipne.ro

Server Name	mdqc01.hpc64.nipne.ro
Server State	Active
Managers	itvasile@mdqc01.hpc64.nipne.ro
Operators	itvasile@mdqc01.hpc64.nipne.ro,paralel@mdqc01.hpc64.nipne.ro
Default Queue	default
State Count	Transit:0 Queued:0 Held:0 Waiting:0 Running:242 Exiting:0
PBS Version	2.3.2

Close

ISyMAB job management – cont (5)



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ISyMAB

Logout

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	34:54:				
1036-236.mdqc01	mirs-job-236	oulas	42:15:				
1036-235.mdqc01	mirs-job-235	oulas	43:18:				
1036-234.mdqc01	mirs-job-234	oulas	32:12:				
1036-233.mdqc01	mirs-job-233	oulas	36:59:	Queue			
1036-232.mdqc01	mirs-job-232	oulas	41:21:	Queue Type			
1036-231.mdqc01	mirs-job-231	oulas	36:18:	Priority		Trans	
				State Count			

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

view the running jobs
and the details for
each queue and each
job

ISyMAB settings and statistics (6)



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Execute NFS
Mount NFS

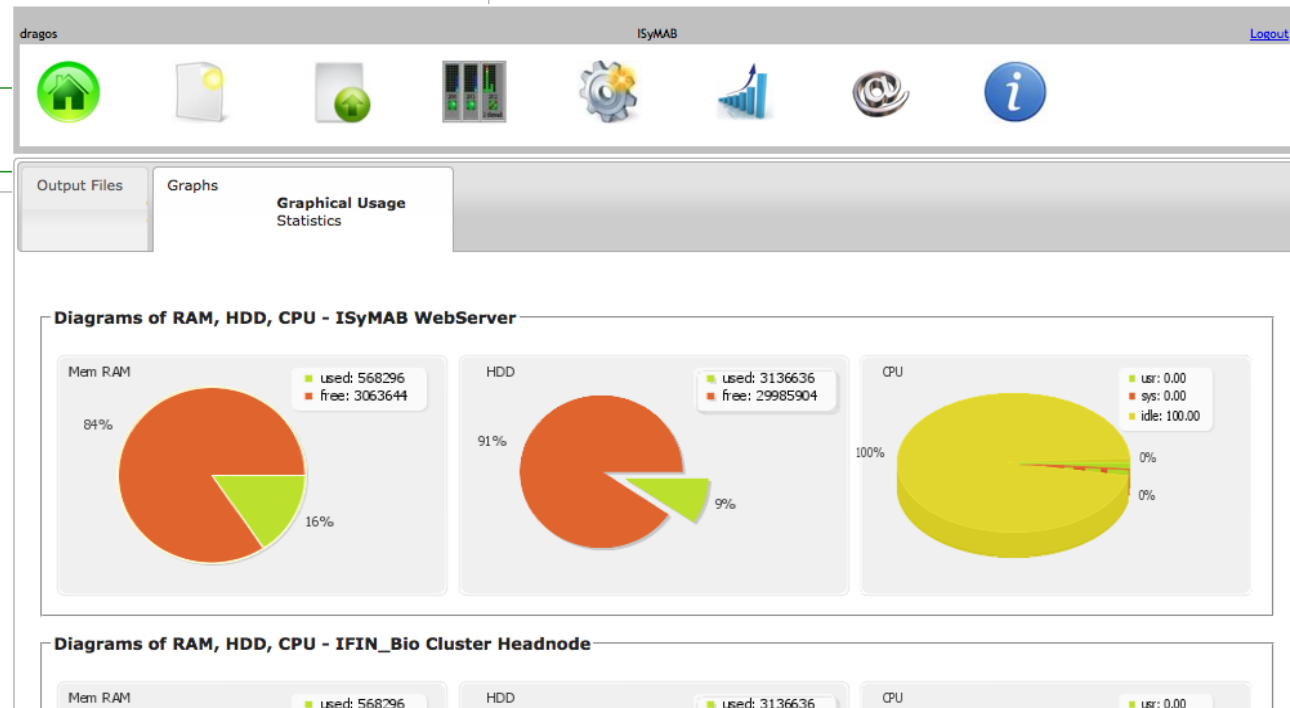
VNC

Mount

Umount

Running...
Mount point - OK

- check settings for NFS file sharing and VNC server
- check statistical graphs



ISyMAB MMTSB package (7)



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ISyMAB Settings

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Create Files
In this area you can edit file.

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

ISyMAB MMTSB – some functions (8)



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ISyMAB Settings

Browser address bar: nipne.ro https://roc.nipne.ro:10110/new/run.php?do_preparation=preparation#tabs-1

ISyMAB Settings

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 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] [-addres 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”.

ISyMAB MMTSB – some functions (9)



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ISyMAB Settings

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.

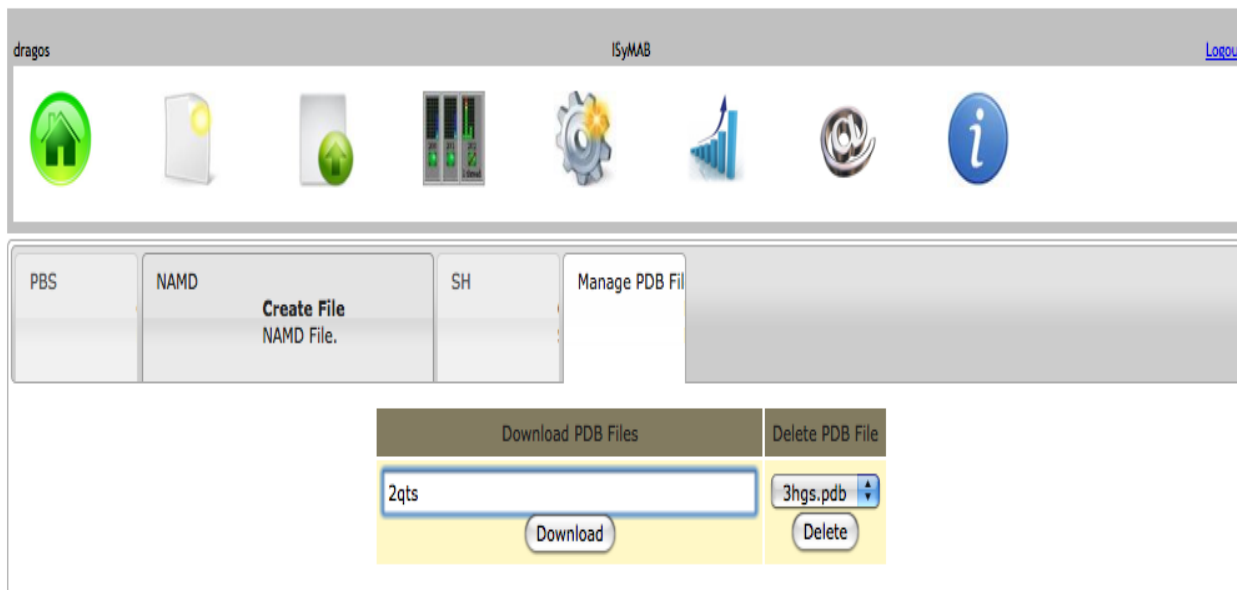
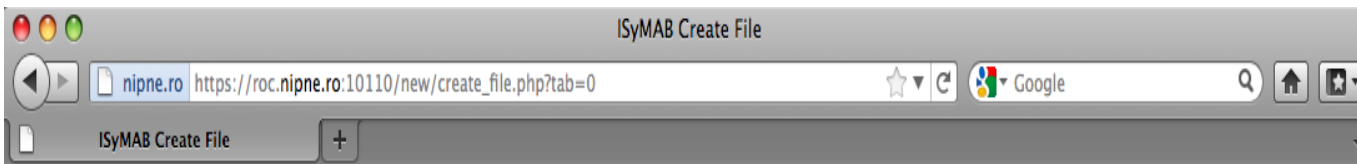
The output files can then be found in the working directory, using the integrated file manager.

ISyMAB download PDB (10)



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We integrated the option to download it directly from RCSB database, using PDB ID.

Prior to this, the PDB files could only be uploaded from one's computer to the IsyMAB server.

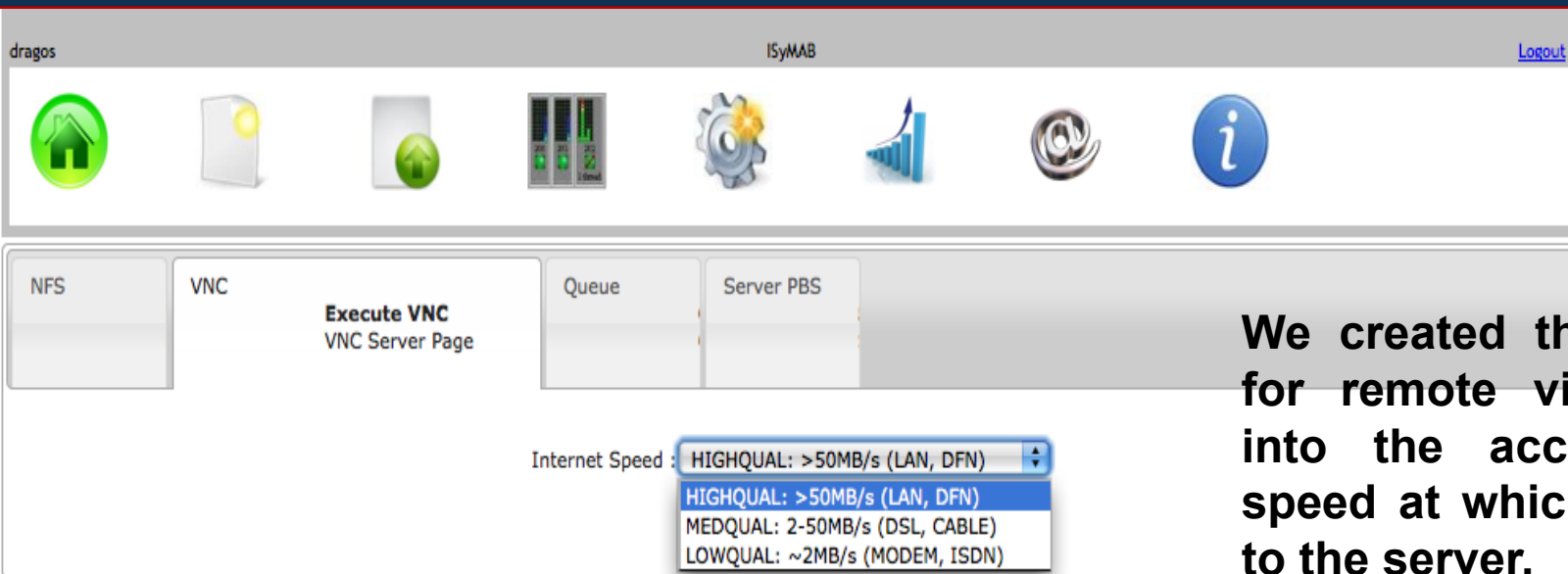
https://roc.nipne.ro:10110/new/create_file.php?tab=0#ui-tabs-2

ISyMAB remote visualization (11)

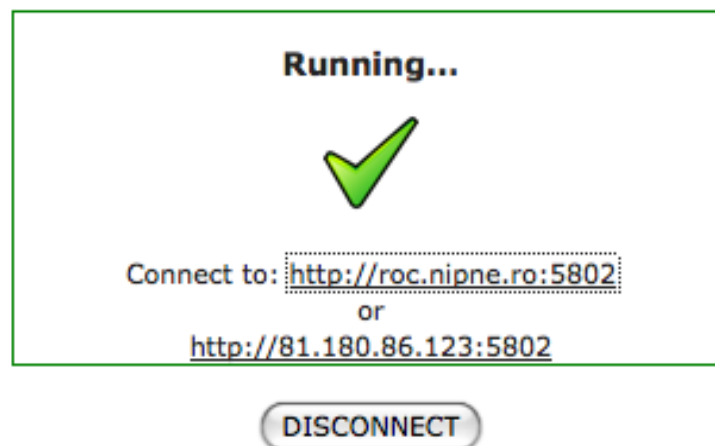


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We created three session types for remote visualization, taking into the account the Internet speed at which you can connect to the server.



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 – cont (12)



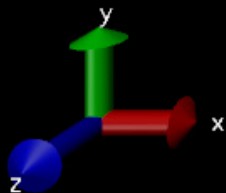
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VMD 1.9 OpenGL Display

VMD

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



ISyMAB remote visualization – cont (13)



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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

Material

Secondary Stri

Opaque

Drawing Method

NewCartoon

Default

Spline Style Catmull-Rom

Aspect Ratio 4.10

Thickness 0.30

Resolution 10



Conclusions and near future prospects

Although of moderate dimensions, the clusters built at IFIN-HH are important for smaller scale research, teaching and training future specialists in parallel computing and new HPC technologies.

Near Future: grid enabled MPI cluster (with gLite 3.2)

Thank you!