HPC Resources Management Portal with Job Scheduler and Load Balancer based on High Throughput Condor : Molecular Dynamics Case Study

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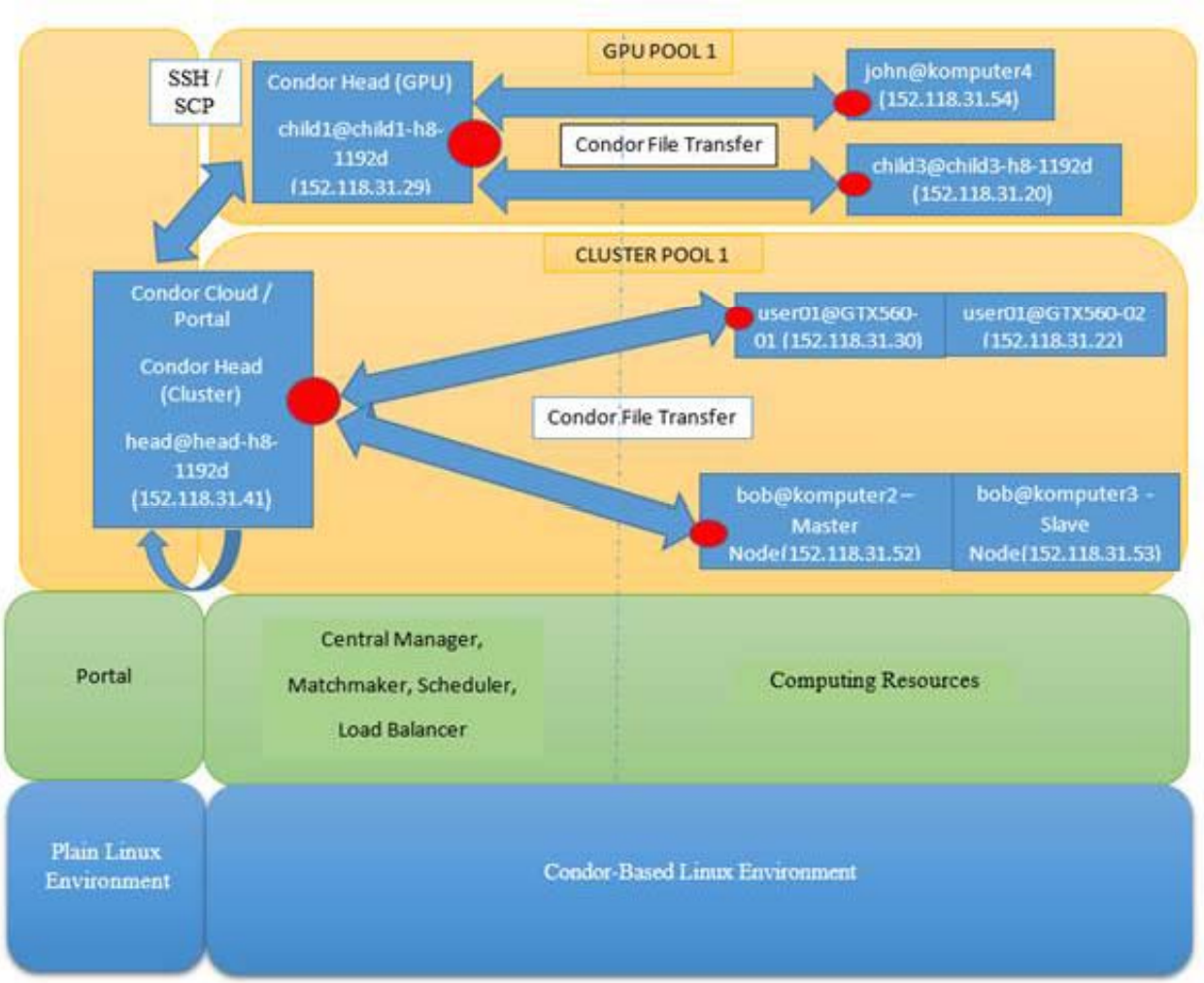
backgrounds

- **Part/The continuation of the work of the development of high performance computing environtment to support computer drug design based on Indonesian medical plant.**
- **Objectives : reliable, affordable, efficient, friendly computing environment**

The proposed architecture



Information of the architecture

- *Condor Portal*: is a PC without condor installed, the connection with the two condor head nodes via SSH. This portal is just an XAMPP server. We plan it is for users to submit the jobs via web services. The red circle indicates where Condor are installed.

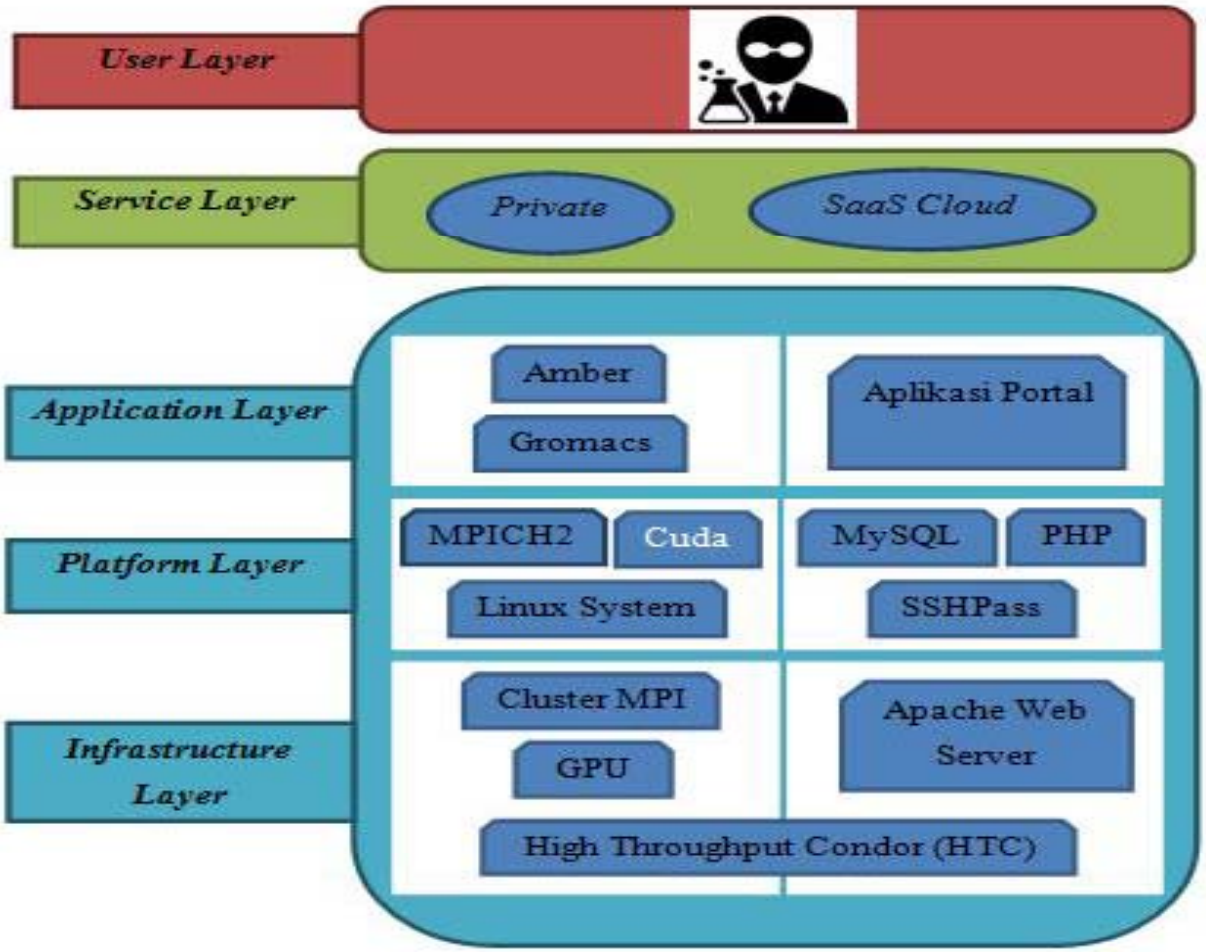
  Condor Heads : function as a Matchmaker, a Central Manager, a Scheduler. All jobs are submitted through these heads. On these, condor are installed. Each of these heads are as follow

- 1). 152.118.31.29: as condor head for pools consisting of GPU resources of two PCs, a and b with one GPU in each . In this head, softwares/applications installed are CUDA, gromacs running on GPU machine.
- a.) 152.118.31.20, it functions as the computing node, condor is installed in it. Also CUDA, gromacs untuk GPU.
- b.) 152.118.31.54, it functions as the computing node, condor is installed in it. Also CUDA, gromacs untuk GPU, amber untuk GPU

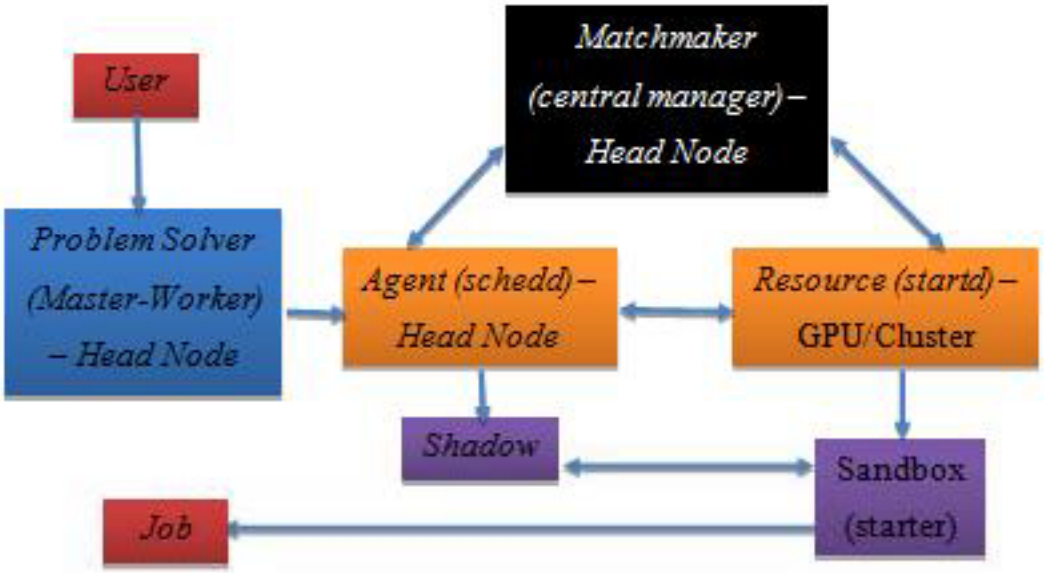
Details of the hosts

Roles	Pool	*IP addresses*	Has HTC ?	Installed applications
Condor Portal	-	152.118.31.41	No	XAMPP Server
Head Node (Matchmaker, Central Manager, Scheduler)	Cluster	152.118.31.41	Yes	mpich2, Gromacs berbasis MPI
	GPU	152.118.31.29	Yes	CUDA, GPU based Gromacs
Resources Node	Cluster	152.118.31.52	Yes	mpich2, MPI based Gromacs, MPI based Amber
		152.118.31.53	No	mpich2, MPI based Gromacs, MPI based Amber
	Cluster	152.118.31.30	Yes	mpich2, MPI based Gromacs
		152.118.31.22	No	mpich2, MPI based Gromacs
	GPU	152.118.31.20	Yes	CUDA, GPU based Gromacs
	GPU	152.118.31.54	Yes	CUDA, GPU based Gromacs, MPI based Gromacs berbasis MPI

The platform design of the portal, head and computing nodes in each pool



Architecture of head node system based on HT Condor



Gambar 3.7 Condor System main Process

Reference : Thain, Douglas, Todd Tannenbaum, dan Miron Livny. (2003). Condor and the Grid (halaman 305). Grid Computing: Making The Global Infrastructure a Reality, 299-335 (reworked)

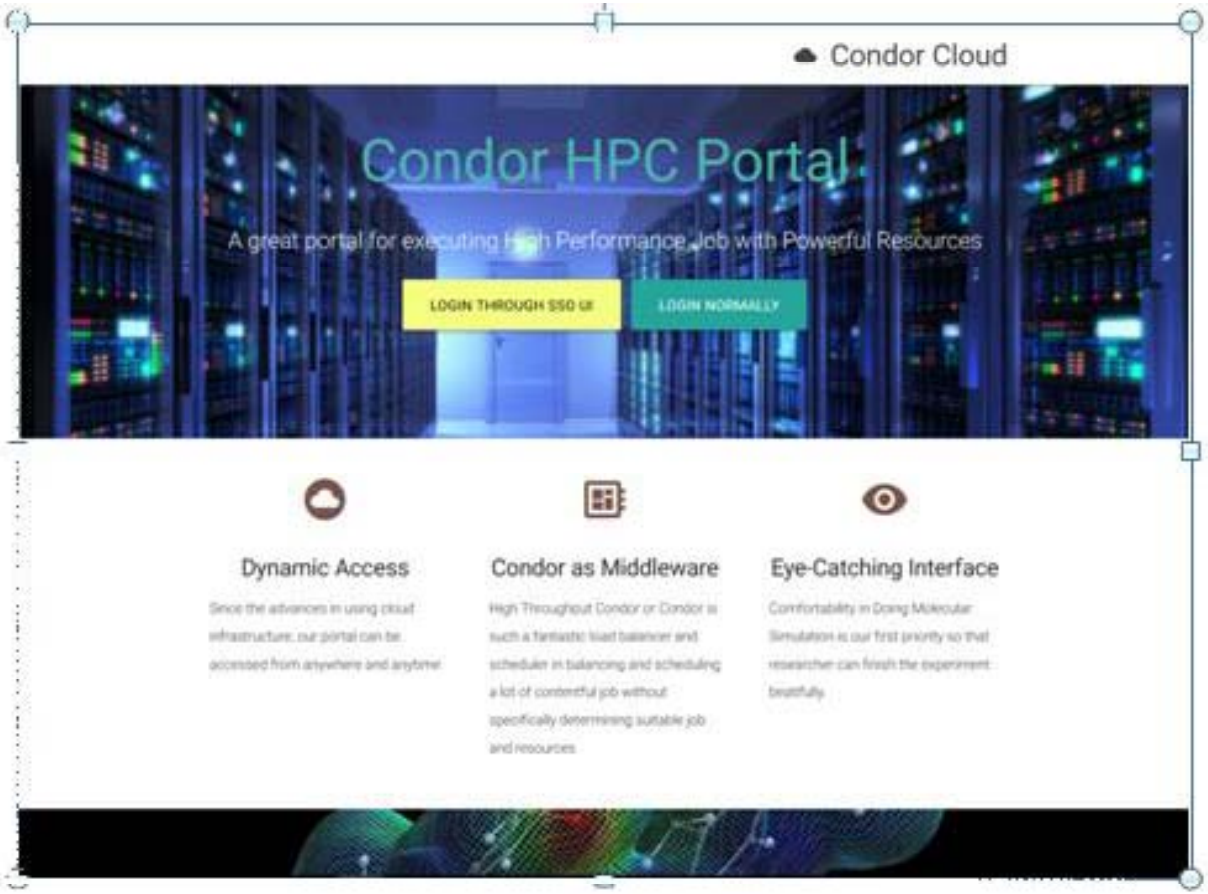
Front End implementation tools

- HTML 5;
- CSS 3;
- JavaScript 1.5;
- JQuery 3.1.1 (*library* as JavaScript *Framework*);
- Materialize CSS 0.97.8 (*library* as CSS *Framework*).

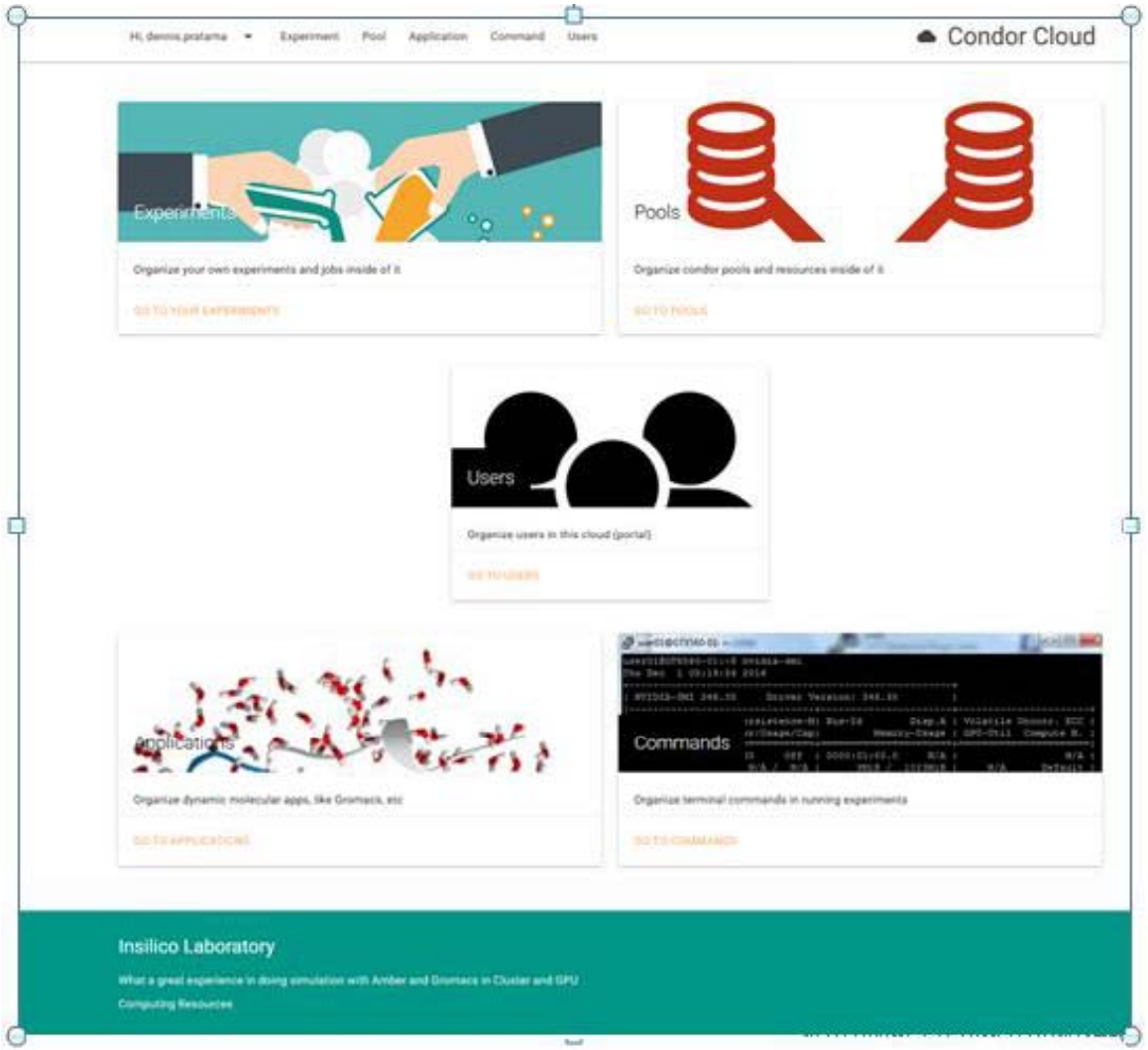
Back End Implementation tools

- PHP 7.0.9
- SSH Pass and shell_exec() function,
- Linux command to terminal
  - sshpass –p “[password]” ssh –o StrictHostKeyChecking=no [username]@[hostname/ IP address] [the_command]
- Copying and moving files
  - sshpass –p “[password]” scp [file to be transferred] [username]@[hostname/IP address]:[path of destination file]

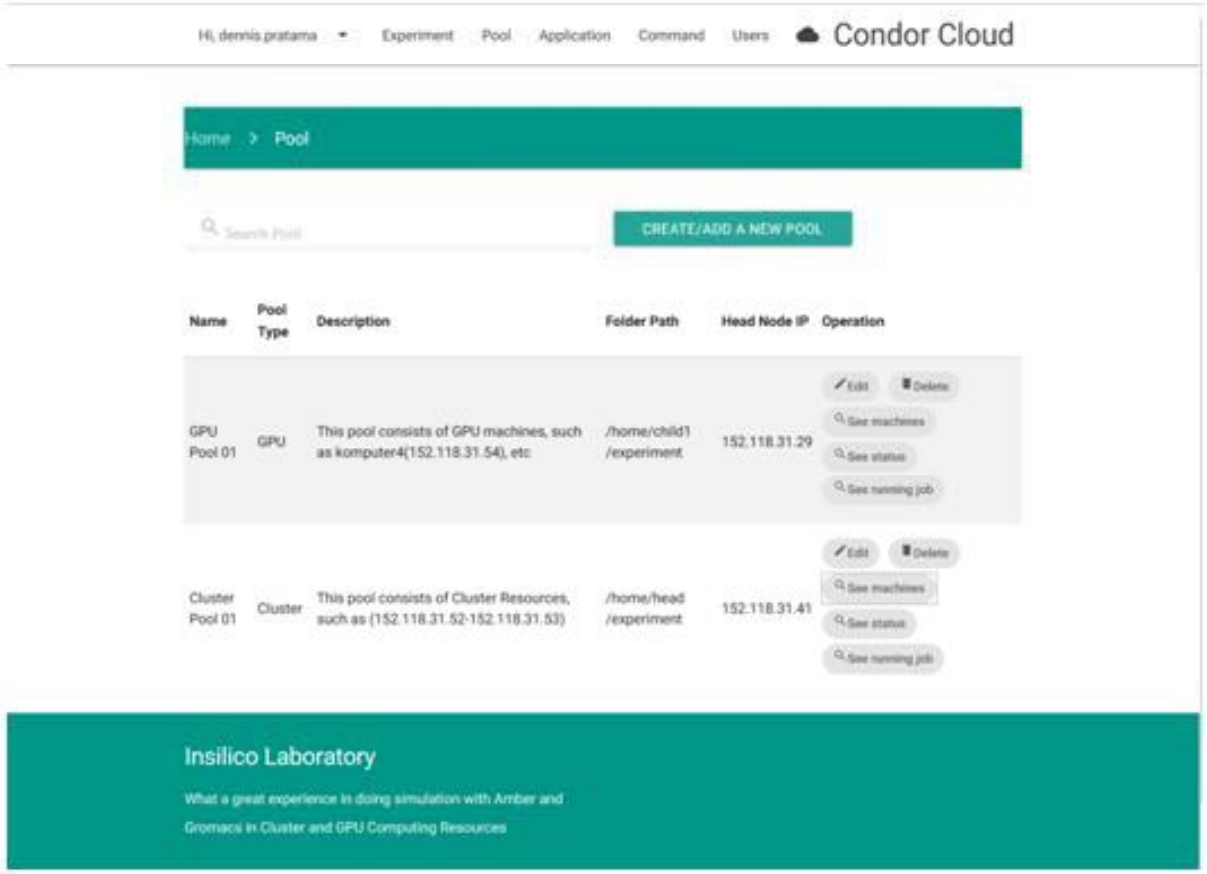
Main page portal



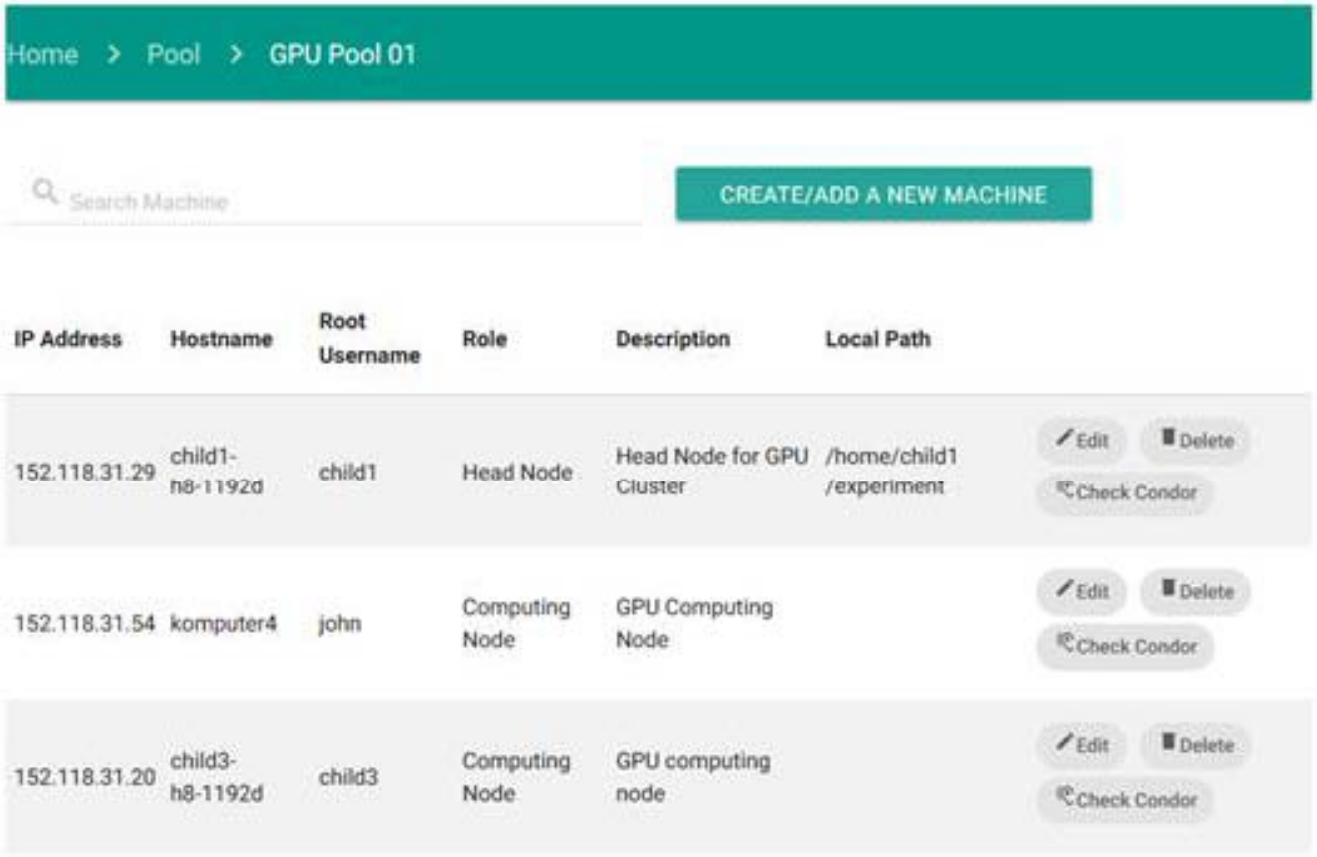
After login view



Pool View


Hi, dennis.pratama
Experiment
Pool
Application
Command
Users
Condor Cloud
Home > Pool
CREATE/ADD A NEW POOL
Name
Pool Type
Description
Folder Path
Head Node IP
Operation
GPU Pool 01
GPU
This pool consists of GPU machines, such as komputer4(152.118.31.54), etc
/home/child1 /experiment
152.118.31.29
Edit
Delete
See machines
See status
See running job
Cluster Pool 01
Cluster
This pool consists of Cluster Resources, such as (152.118.31.52-152.118.31.53)
/home/head /experiment
152.118.31.41
Insilico Laboratory
What a great experience in doing simulation with Amber and Gromacs in Cluster and GPU Computing Reaources

GPU pool view

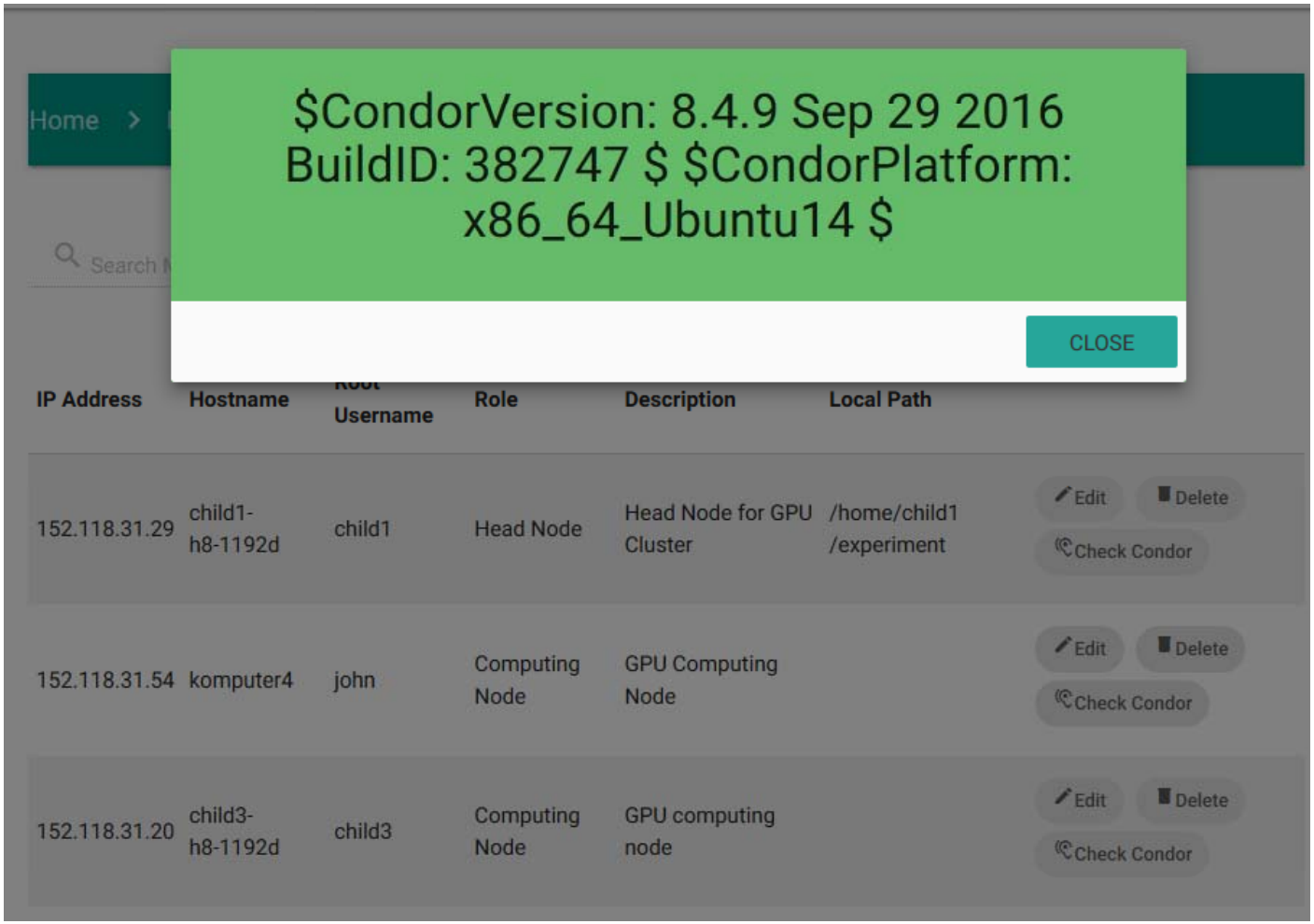


Resources Node and Its Slots located in this pool

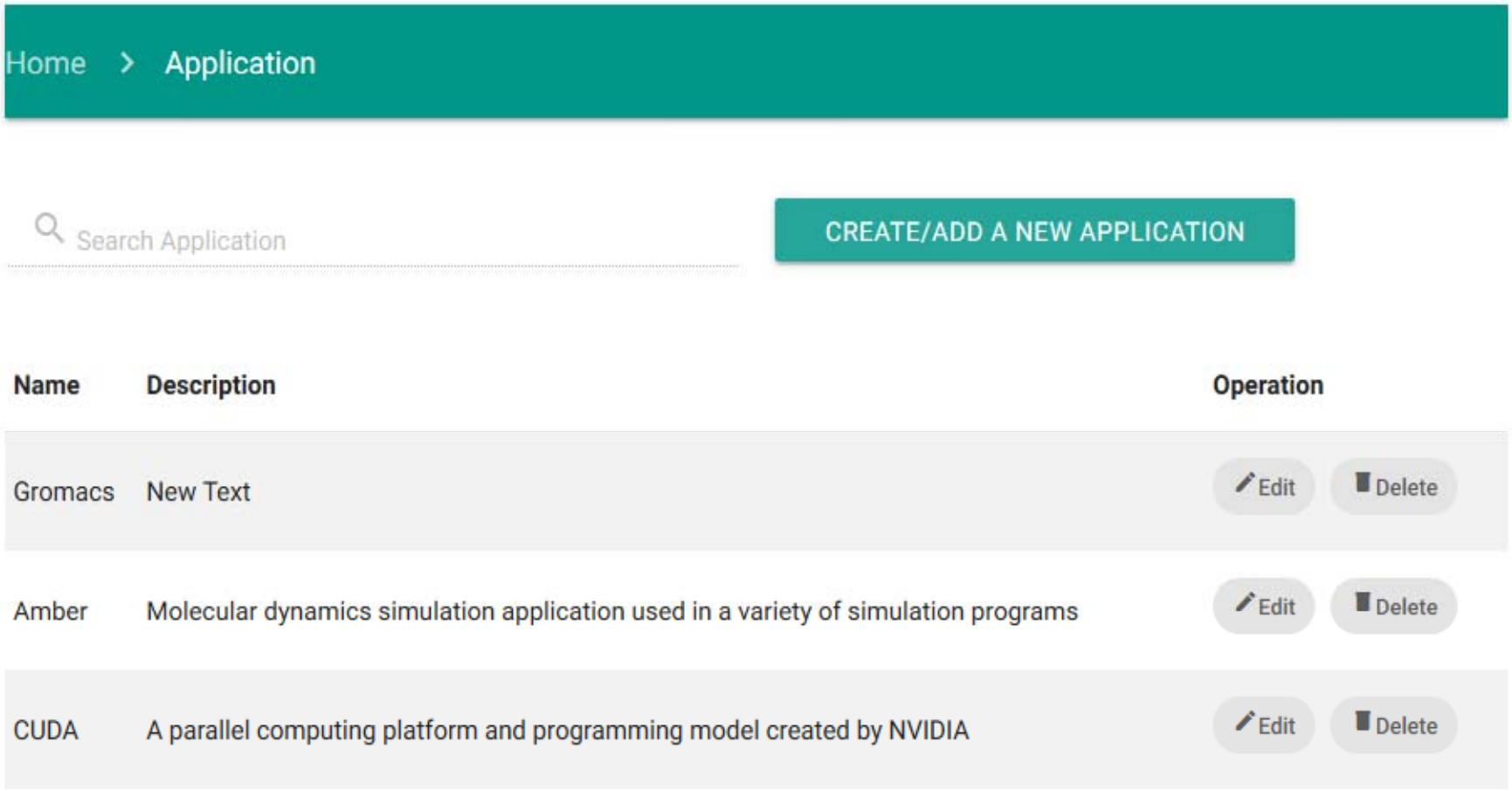
Name	Operating System	Architecture	State	Activity	Load Average	Memory	Activity Time
slot1@child3-h8-11	LINUX	X86_64	Unclaimed	Idle	0.000	743	2+19:41:17
slot2@child3-h8-11	LINUX	X86_64	Unclaimed	Idle	0.000	743	3+16:03:46
slot3@child3-h8-11	LINUX	X86_64	Unclaimed	Idle	0.010	743	9+21:12:08
slot4@child3-h8-11	LINUX	X86_64	Unclaimed	Idle	0.000	743	9+21:12:09
slot5@child3-h8-11	LINUX	X86_64	Unclaimed	Idle	0.000	743	9+21:12:10
slot6@child3-h8-11	LINUX	X86_64	Unclaimed	Idle	0.000	743	9+21:12:11
slot7@child3-h8-11	LINUX	X86_64	Unclaimed	Idle	0.000	743	9+21:12:12
slot8@child3-h8-11	LINUX	X86_64	Unclaimed	Idle	0.000	743	9+21:12:05
slot1@komputer4	LINUX	X86_64	Unclaimed	Idle	0.000	743	1+15:49:50
slot2@komputer4	LINUX	X86_64	Unclaimed	Idle	0.000	743	1+15:50:20
slot3@komputer4	LINUX	X86_64	Unclaimed	Idle	0.000	743	1+15:50:21
slot4@komputer4	LINUX	X86_64	Unclaimed	Idle	0.000	743	1+15:50:22
slot5@komputer4	LINUX	X86_64	Unclaimed	Idle	0.000	743	1+15:50:23
slot6@komputer4	LINUX	X86_64	Unclaimed	Idle	0.000	743	1+15:50:24
slot7@komputer4	LINUX	X86_64	Unclaimed	Idle	0.000	743	1+15:50:25
slot8@komputer4	LINUX	X86_64	Unclaimed	Idle	0.000	743	1+15:50:18
	Total	Owner	Claimed	Unclaimed	Matched	Preempting	Backfill
	X86_64/LINUX	16	0	0	16	0	0
	Total	16	0	0	16	0	0

REFRESH BACK TO PREVIOUS

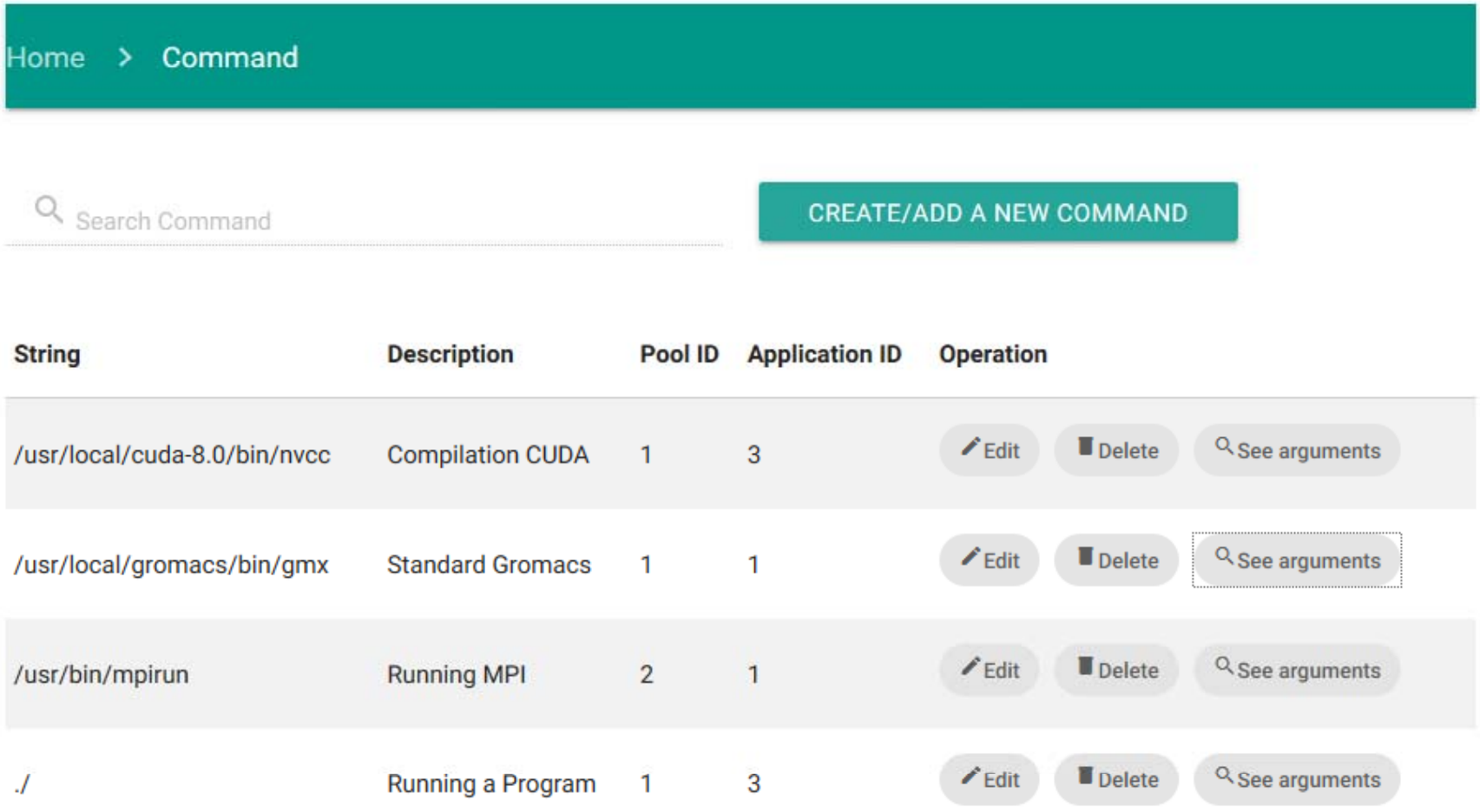
Checking Condor installed



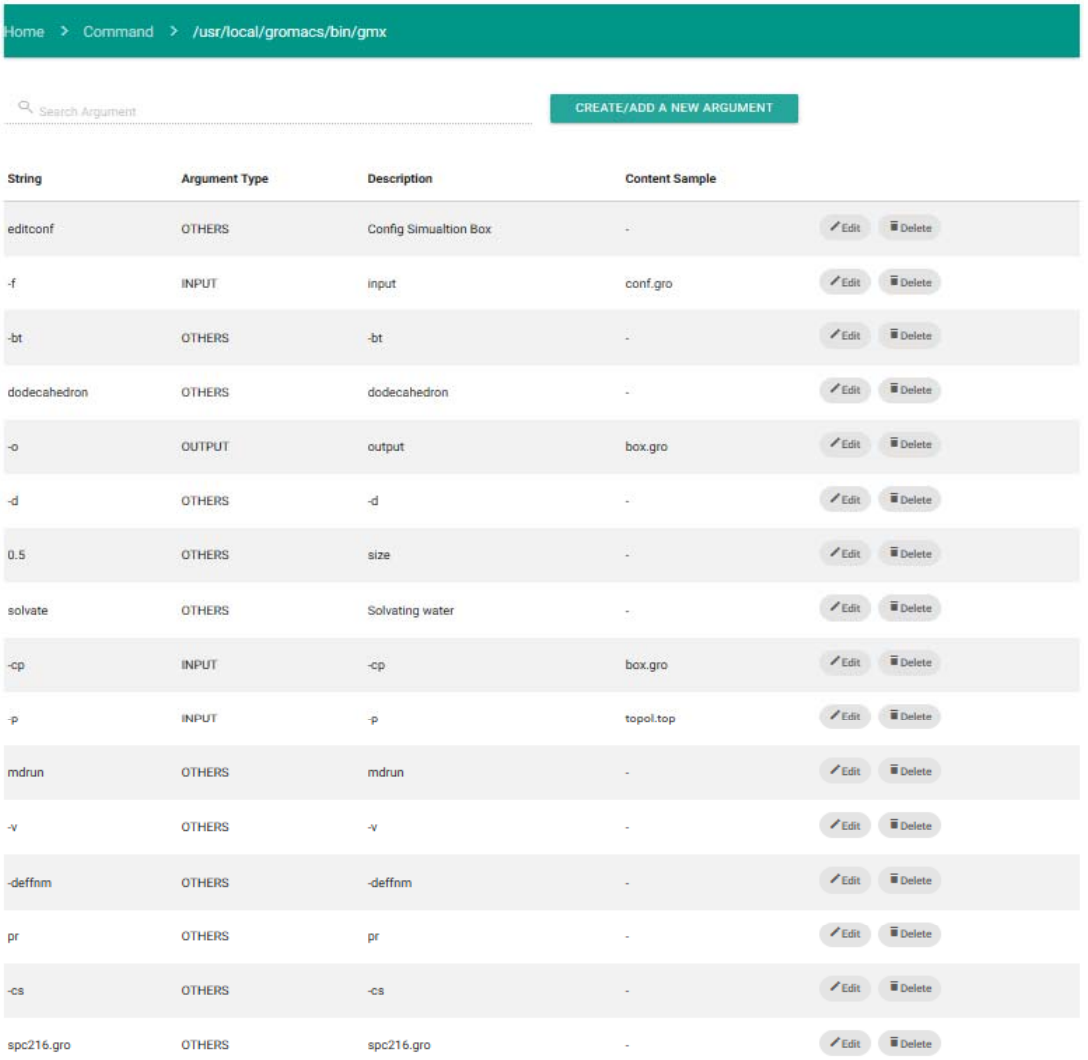
Applications installed



Commands installed

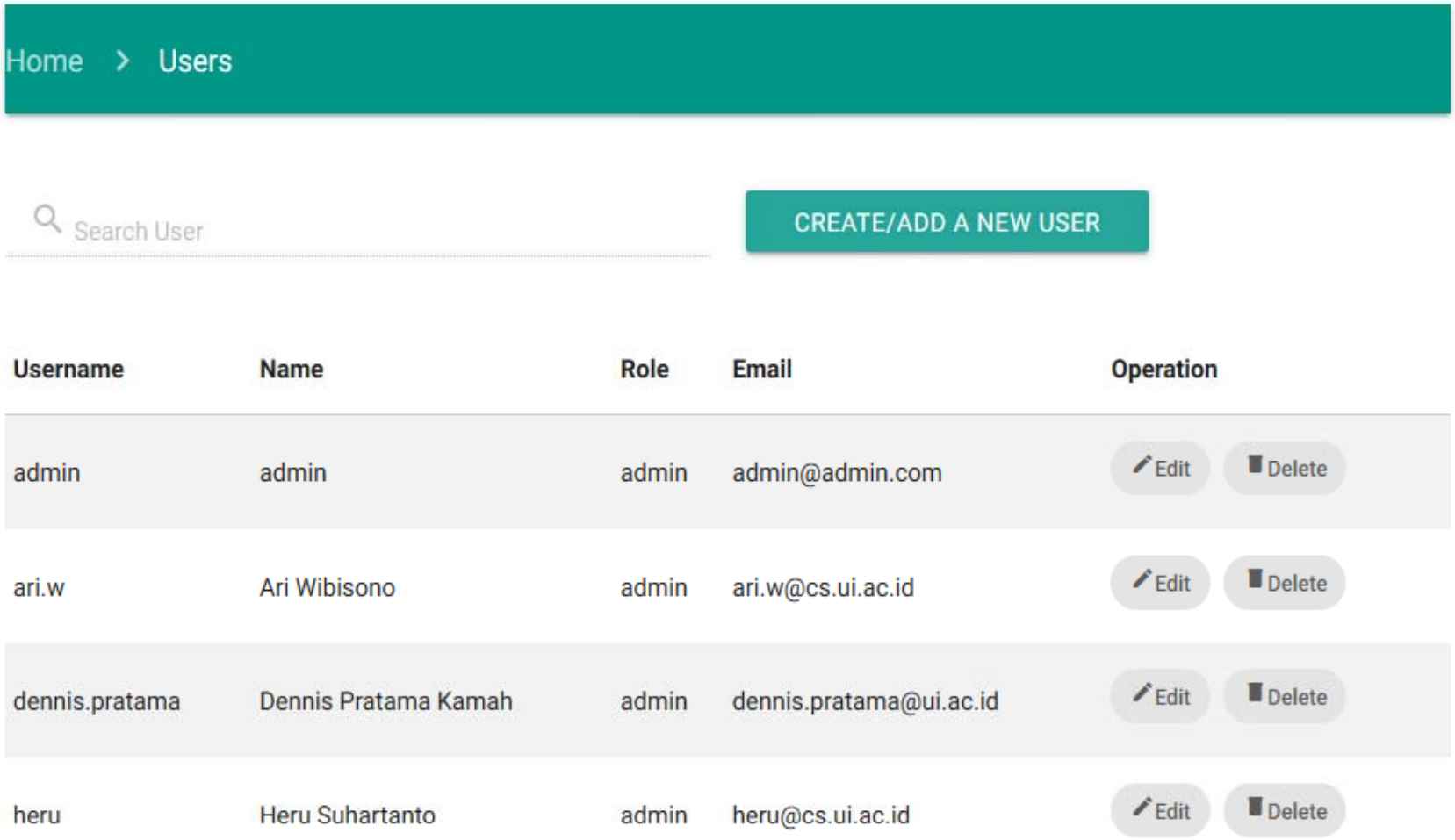


Arguments in *Command* “/usr/local/gromacs/bin/gmx”



String	Argument Type	Description	Content Sample	
editconf	OTHERS	Config Simualtion Box	-	Edit Delete
-f	INPUT	input	conf.gro	Edit Delete
-bt	OTHERS	-bt	-	Edit Delete
dodecahedron	OTHERS	dodecahedron	-	Edit Delete
-o	OUTPUT	output	box.gro	Edit Delete
-d	OTHERS	-d	-	Edit Delete
0.5	OTHERS	size	-	Edit Delete
solvate	OTHERS	Solvating water	-	Edit Delete
-cp	INPUT	-cp	box.gro	Edit Delete
-p	INPUT	-p	topol.top	Edit Delete
mdrun	OTHERS	mdrun	-	Edit Delete
-v	OTHERS	-v	-	Edit Delete
-deffnm	OTHERS	-deffnm	-	Edit Delete
pr	OTHERS	pr	-	Edit Delete
-cs	OTHERS	-cs	-	Edit Delete
spc216.gro	OTHERS	spc216.gro	-	Edit Delete

Registered users



Create New Experiment

User ID

dennis.pratama

Pool ID

GPU Pool 01

Application ID

Gromacs

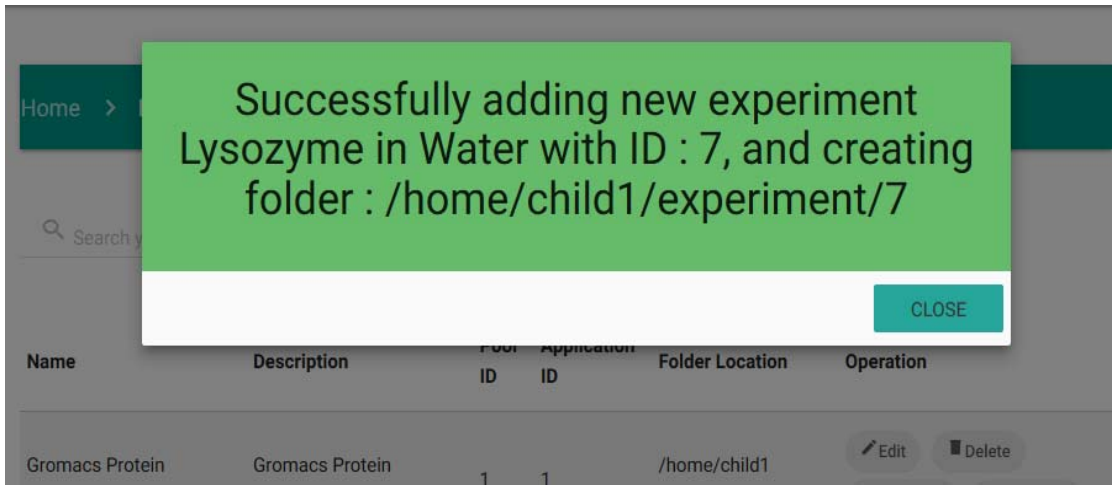
Experiment Name

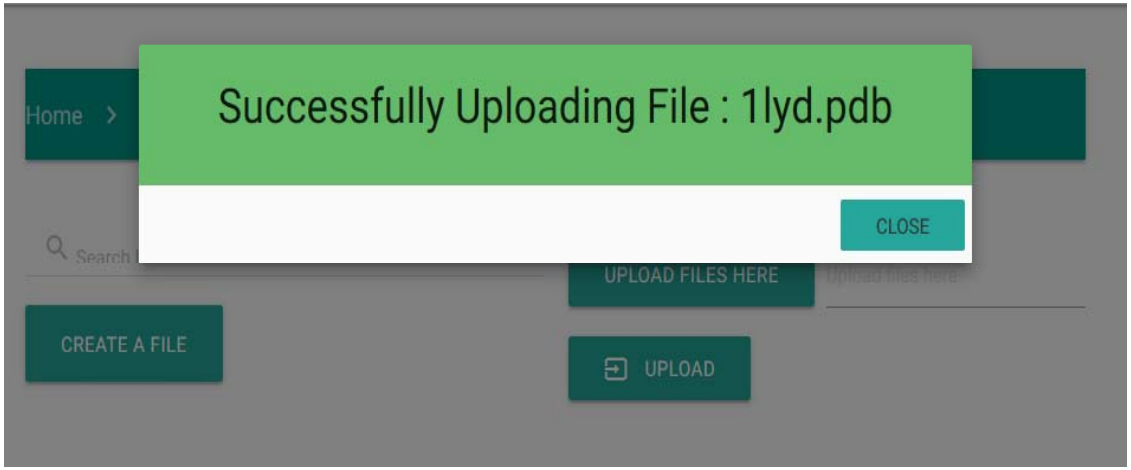
Lysozyme in Water

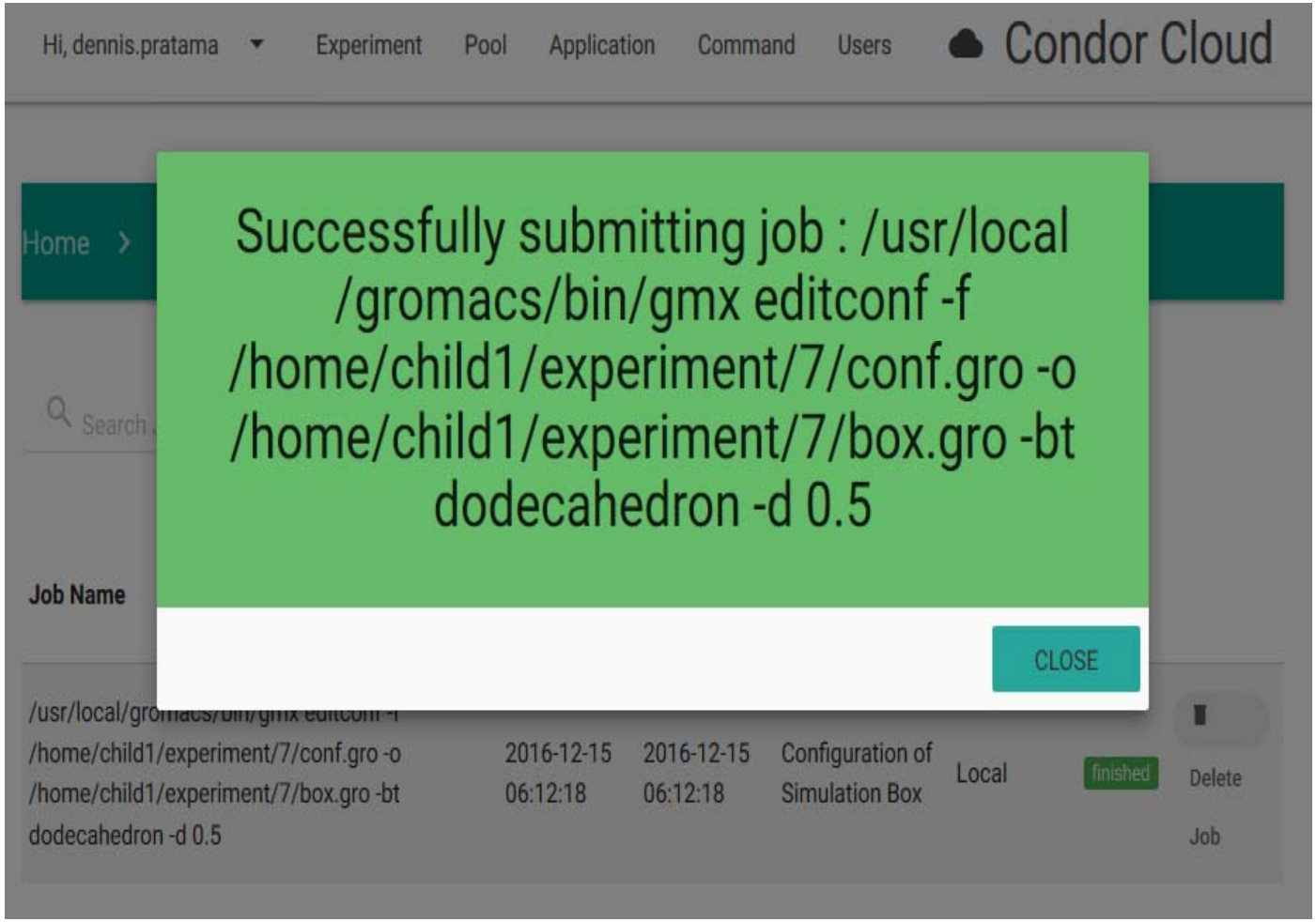
Experiment Description

Lysozyme in Water

CREATE


Home
Search y
Successfully adding new experiment Lysozyme in Water with ID : 7, and creating folder : /home/child1/experiment/7
CLOSE
Name
Description
ID
ID
Folder Location
Operation
Gromacs Protein
Gromacs Protein
1
1
/home/child1
Edit
Delete


Home
Search
Successfully Uploading File : 1lyd.pdb
CLOSE
UPLOAD FILES HERE
CREATE A FILE
UPLOAD


Hi, dennis.pratama
Experiment
Pool
Application
Command
Users
Condor Cloud
Home
Search
Job Name
Successfully submitting job : /usr/local /gromacs/bin/gmx editconf -f /home/child1/experiment/7/conf.gro -o /home/child1/experiment/7/box.gro -bt dodecahedron -d 0.5
CLOSE
/home/child1/experiment/7/conf.gro -o /home/child1/experiment/7/box.gro -bt dodecahedron -d 0.5
2016-12-15 06:12:18
2016-12-15 06:12:18
Configuration of Simulation Box
Local
finished
Delete Job

Files after submition

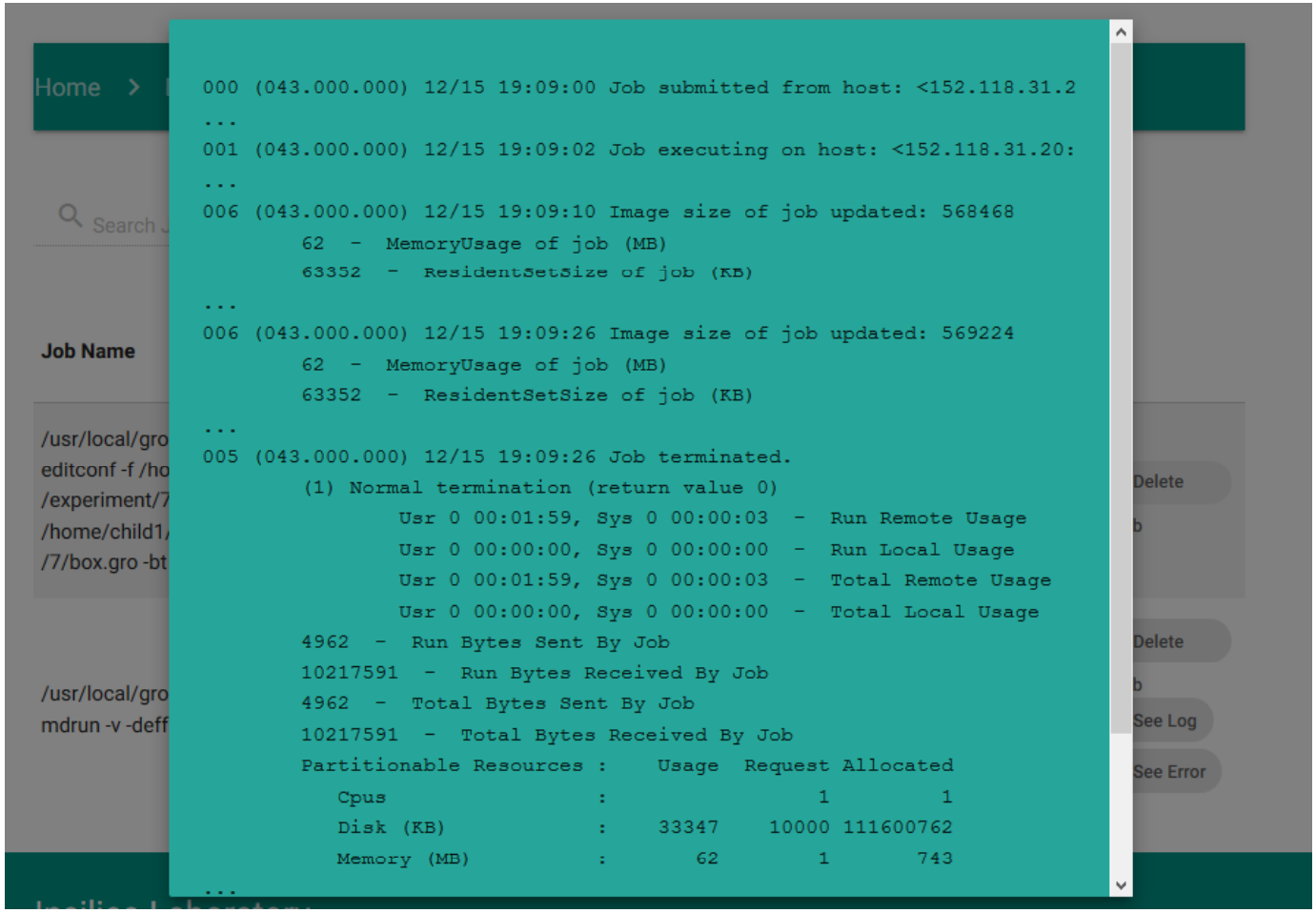
Files located in folder : /home/child1/experiment/7

Name	Permissions	User	Group	Size (in byte)	Last Modified	File Operations
1lyd.pdb	-rw-r--r--	child1	child1	144909	Des 15, 18:19	DOWNLOAD FILE VIEW FILE DELETE FILE
box.gro	-rw-rw-r--	child1	child1	130114	Des 15, 18:46	DOWNLOAD FILE VIEW FILE DELETE FILE
conf.gro	-rw-rw-r--	child1	child1	130114	Des 15, 18:45	DOWNLOAD FILE VIEW FILE DELETE FILE
posre.itp	-rw-rw-r--	child1	child1	40852	Des 15, 18:45	DOWNLOAD FILE VIEW FILE DELETE FILE
topol.top	-rw-rw-r--	child1	child1	775772	Des 15, 18:45	DOWNLOAD FILE VIEW FILE DELETE FILE

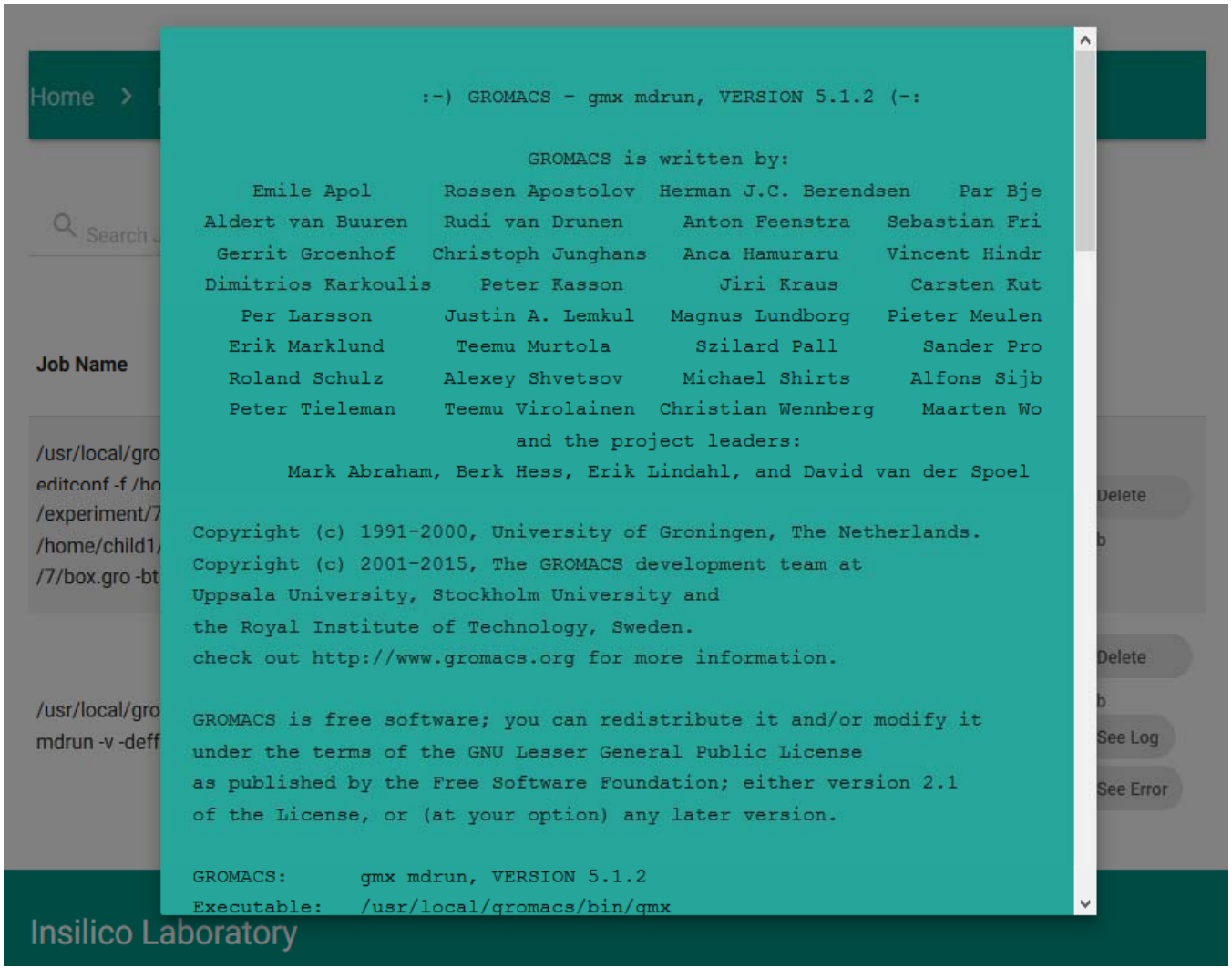
Finished jobs

Job Name	Condor ID	Starting Time	Finished Time	Description	Execution	Status	
/usr/local/gromacs/bin/gmx editconf -f /home/child1 /experiment/7/conf.gro -o /home/child1/experiment /7/box.gro -bt dodecahedron -d 0.5		2016-12-15 06:12:18	2016-12-15 06:12:18	Configuration of Simulation Box	Local	finished	Delete Job
/usr/local/gromacs/bin/gmx mdrun -v -deffnm pr	43	2016-12-15 19:09:00	2016-12-15 19:09:26	Water Equilibration	Remote	finished	Delete Job See Log See Error

Log of jobs with HTC



Job Output with HTC



Machines status and Slot in GPU pool

Name	Operating System	Architecture	State	Activity	Load Average	Memory	Activity Time
slot1@child3-h8-11	LINUX	X86_64	Claimed	Busy	0.000	743	0+00:00:04
slot2@child3-h8-11	LINUX	X86_64	Claimed	Busy	0.000	743	0+00:00:05
slot3@child3-h8-11	LINUX	X86_64	Claimed	Busy	0.000	743	0+00:00:06
slot4@child3-h8-11	LINUX	X86_64	Claimed	Busy	0.000	743	0+00:00:07
slot5@child3-h8-11	LINUX	X86_64	Claimed	Busy	0.000	743	0+00:00:08
slot6@child3-h8-11	LINUX	X86_64	Claimed	Busy	0.000	743	0+00:00:09
slot7@child3-h8-11	LINUX	X86_64	Claimed	Busy	0.000	743	0+00:00:10
slot8@child3-h8-11	LINUX	X86_64	Claimed	Busy	0.000	743	0+00:00:03
slot1@komputer4	LINUX	X86_64	Claimed	Busy	0.000	743	0+00:00:04
slot2@komputer4	LINUX	X86_64	Claimed	Busy	0.000	743	0+00:00:05
slot3@komputer4	LINUX	X86_64	Unclaimed	Idle	0.000	743	11+03:46:45
slot4@komputer4	LINUX	X86_64	Unclaimed	Idle	0.000	743	11+03:46:46
slot5@komputer4	LINUX	X86_64	Unclaimed	Idle	0.000	743	11+03:46:47
slot6@komputer4	LINUX	X86_64	Unclaimed	Idle	0.000	743	11+03:46:48
slot7@komputer4	LINUX	X86_64	Unclaimed	Idle	0.000	743	11+03:46:49
slot8@komputer4	LINUX	X86_64	Unclaimed	Idle	0.000	743	11+03:46:42

Machines status and Slot in Cluster pool

Name	Operating System	Architecture	State	Activity	Load Average	Memory	Activity Time
slot1@GTX560-01	LINUX	X86_64	Unclaimed	Idle	1.000	745	11+21:56:27
slot2@GTX560-01	LINUX	X86_64	Unclaimed	Idle	0.060	745	11+21:56:48
slot3@GTX560-01	LINUX	X86_64	Unclaimed	Idle	0.000	745	11+21:56:49
slot4@GTX560-01	LINUX	X86_64	Unclaimed	Idle	0.000	745	11+21:56:50
slot5@GTX560-01	LINUX	X86_64	Unclaimed	Idle	0.000	745	11+21:56:51
slot6@GTX560-01	LINUX	X86_64	Unclaimed	Idle	0.000	745	11+21:56:52
slot7@GTX560-01	LINUX	X86_64	Unclaimed	Idle	0.000	745	11+21:56:53
slot8@GTX560-01	LINUX	X86_64	Unclaimed	Idle	0.000	745	11+21:56:46
slot1@komputer2	LINUX	X86_64	Claimed	Busy	0.000	743	0+00:00:04
slot2@komputer2	LINUX	X86_64	Claimed	Busy	0.000	743	0+00:00:05
slot3@komputer2	LINUX	X86_64	Claimed	Busy	0.000	743	0+00:00:06
slot4@komputer2	LINUX	X86_64	Claimed	Busy	0.000	743	0+00:00:07
slot5@komputer2	LINUX	X86_64	Claimed	Busy	1.000	743	0+00:00:08
slot6@komputer2	LINUX	X86_64	Claimed	Busy	1.000	743	0+00:00:09
slot7@komputer2	LINUX	X86_64	Claimed	Busy	0.000	743	0+00:00:10
slot8@komputer2	LINUX	X86_64	Unclaimed	Idle	0.170	743	0+00:00:02

Conclusions

- The last two pictures shows that load balancing and jobs scheduling are running fine
- In the GPU pool with 10 jobs, slots and jobs are distributed evently, if a slot is filled with a job, the new jobs will be allocated to “idle” slot..
- This shows that HTC could do load balancing well.

Conclusions

- The two figures also show that HTC increase the throughput from available machines where the HTC allocates all available slot first.

- This also happens to the Cluster pool.

Suggestions (Nadya, 170105)

- A condor portal machine is of no interest for a moment as this is merely a host form which users ssh to another condor-enabled hosts.
- Currently there are 2 pools configured and i think they should be combined into one pool and have only one condor head running.