

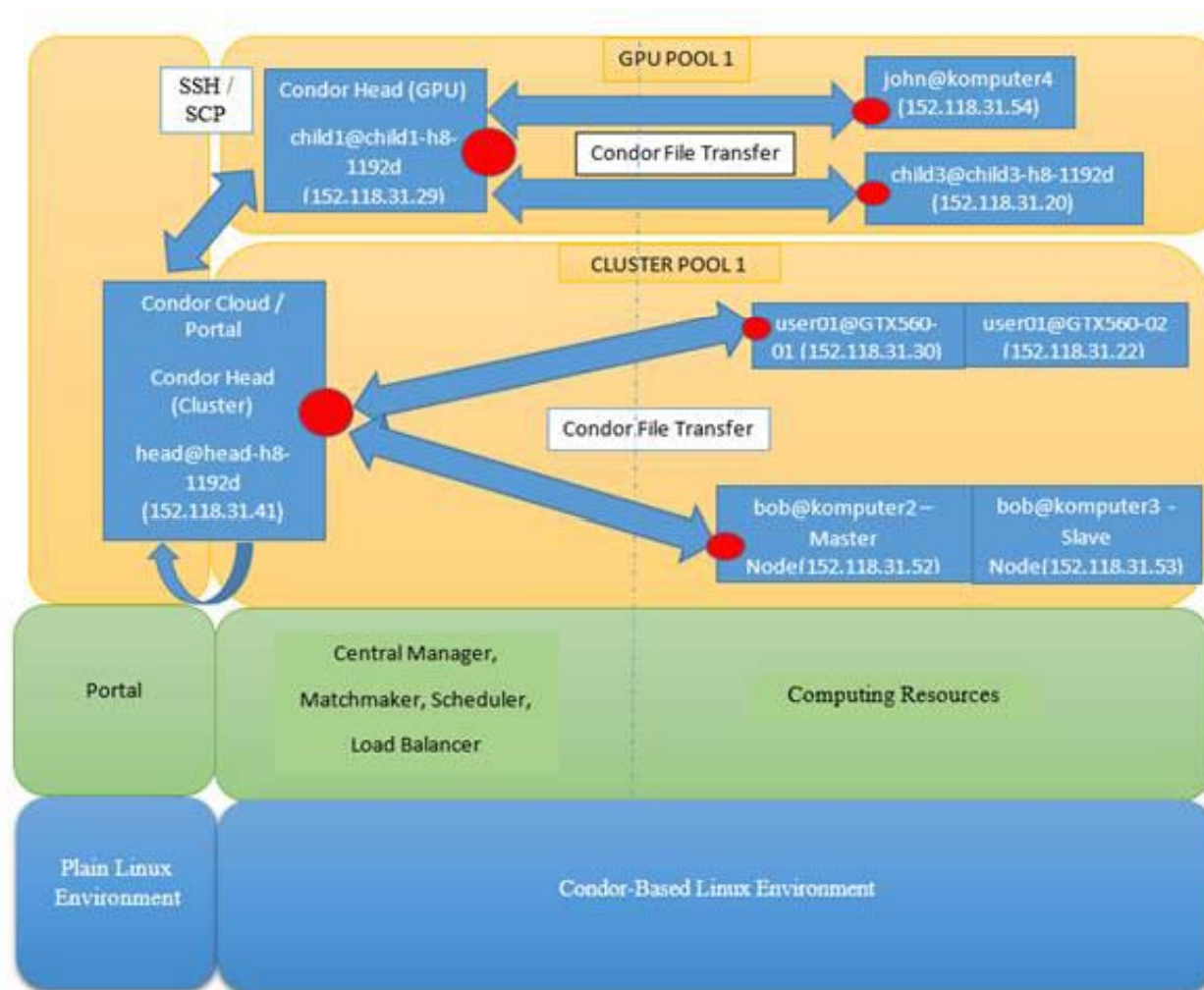
# HPC Resources Management Portal with Job Scheduler and Load Balancer based on High Throughput Condor : Molecular Dynamics Case Study

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# backgrounds

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

# The proposed architecture



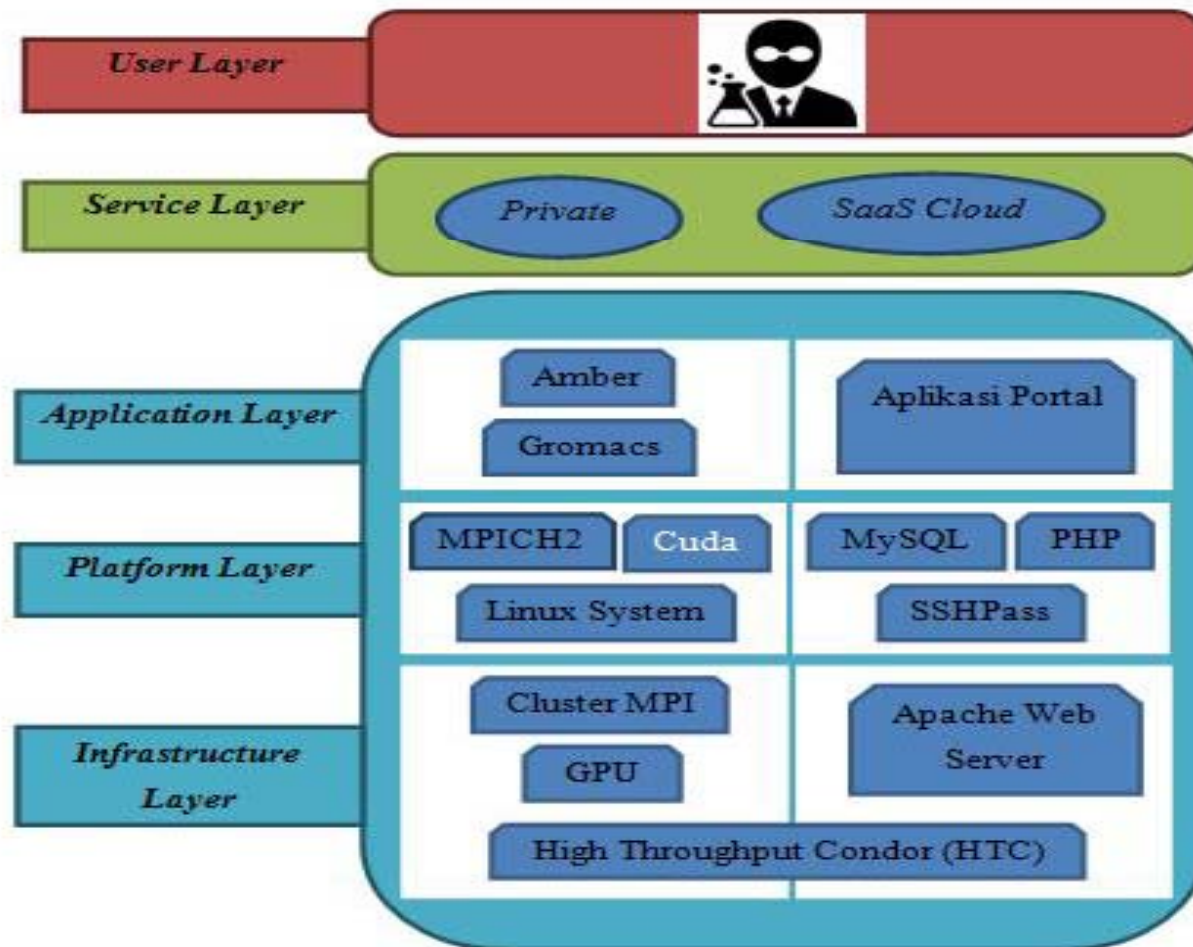
# Information of the architecture

- **\*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

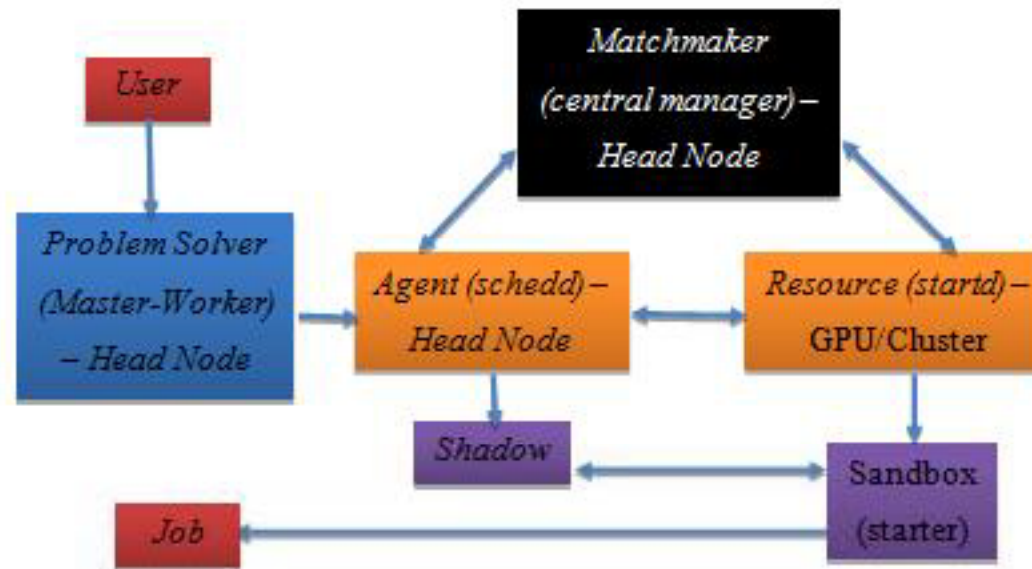
# Details of the hosts

Roles	Pool	IP addresses	Has <u>HTC?</u>	Installed applications
Condor Portal	-	152.118.31.41	No	XAMPP Server
<i>Head Node (Matchmaker, Central Manager, Scheduler)</i>	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

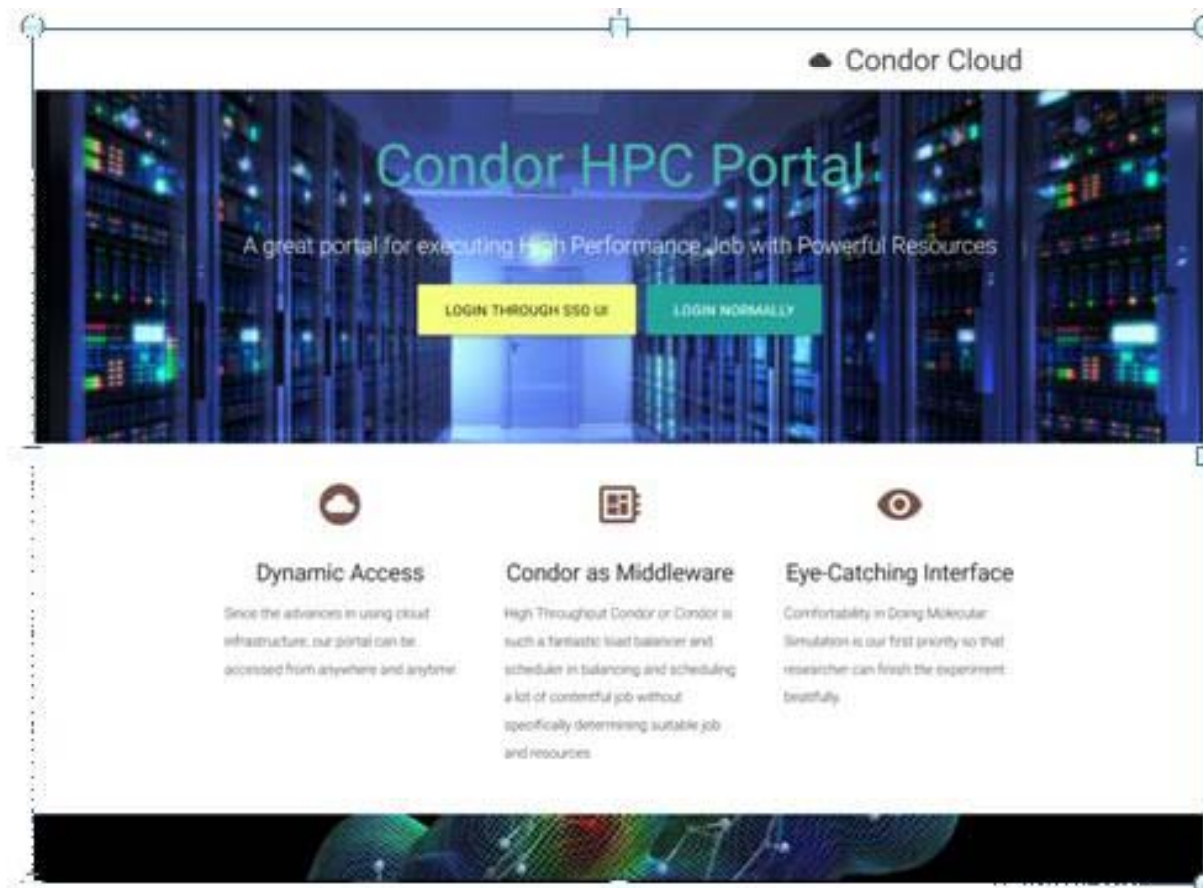
- HTML 5;
- CSS 3;
- JavaScript 1.5;
- JQuery 3.1.1 (*library* as JavaScript *Framework*);
- Materialize CSS 0.97.8 (*library* as CSS *Framework*).



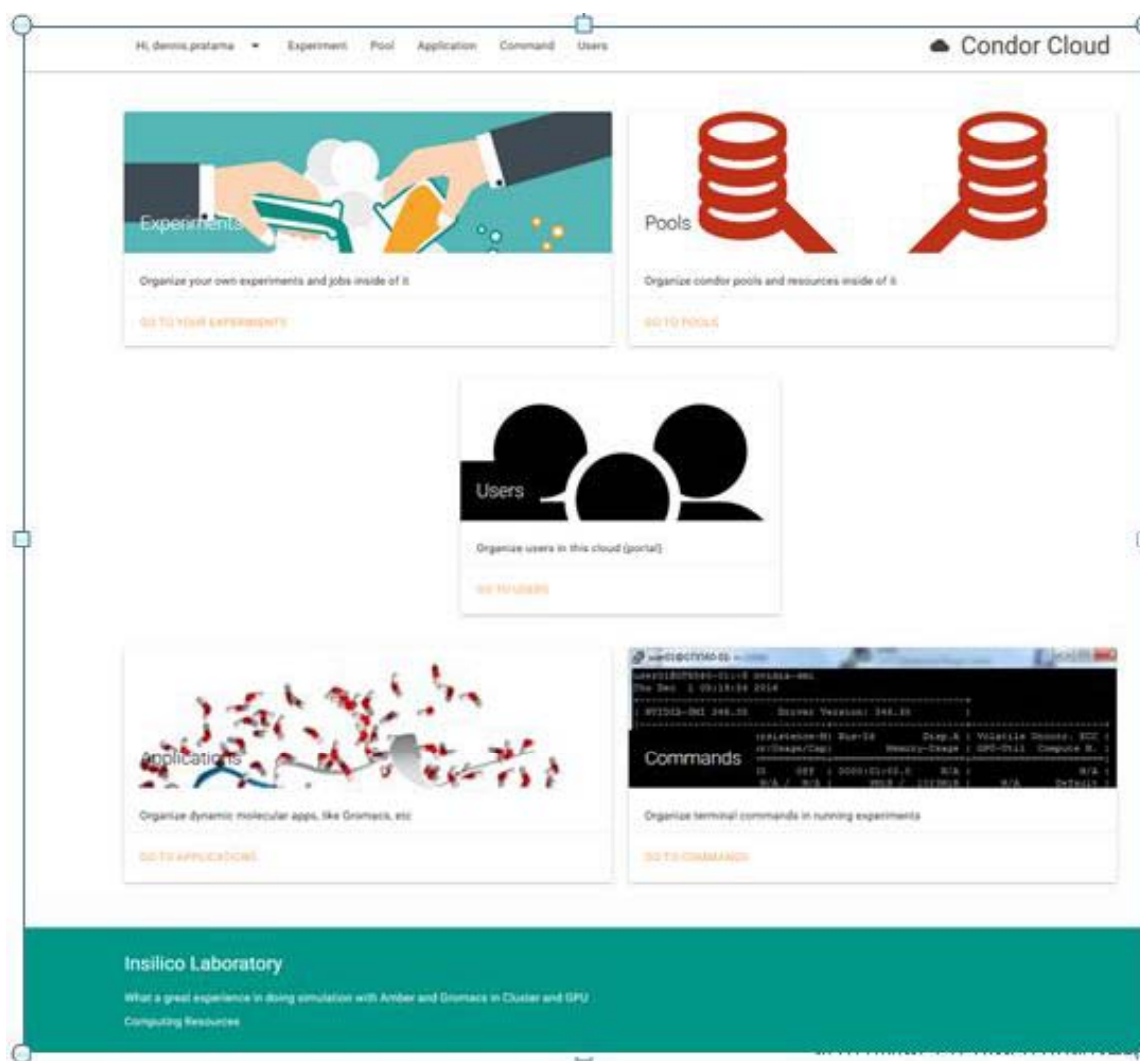
# Back End Implementation tools

- 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

ExperimentPoolApplicationCommandUsers

Condor Cloud

Home > Pool

Search 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	<div><div>EditDelete</div><div>See machines</div><div>See status</div><div>See running job</div></div>
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	<div><div>EditDelete</div><div>See machines</div><div>See status</div><div>See running job</div></div>

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What a great experience in doing simulation with Amber and Gromacs in Cluster and GPU Computing Resources

# GPU pool view

Home > Pool > GPU Pool 01

 Search Machine

CREATE/ADD A NEW MACHINE

IP Address	Hostname	Root Username	Role	Description	Local Path	
152.118.31.29	child1-n8-1192d	child1	Head Node	Head Node for GPU Cluster	/home/child1/experiment	<div><div>Edit</div><div>Delete</div><div>Check Condor</div></div>
152.118.31.54	komputer4	john	Computing Node	GPU Computing Node		<div><div>Edit</div><div>Delete</div><div>Check Condor</div></div>
152.118.31.20	child3-h8-1192d	child3	Computing Node	GPU computing node		<div><div>Edit</div><div>Delete</div><div>Check Condor</div></div>

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

Home >








Search

\$CondorVersion: 8.4.9 Sep 29 2016  
BuildID: 382747 \$ \$CondorPlatform:  
x86\_64\_Ubuntu14 \$

CLOSE

IP Address	Hostname	Root Username	Role	Description	Local Path	
152.118.31.29	child1-h8-1192d	child1	Head Node	Head Node for GPU Cluster	/home/child1/experiment	<a href="#">Edit</a> <a href="#">Delete</a> <a href="#">Check Condor</a>
152.118.31.54	komputer4	john	Computing Node	GPU Computing Node		<a href="#">Edit</a> <a href="#">Delete</a> <a href="#">Check Condor</a>
152.118.31.20	child3-h8-1192d	child3	Computing Node	GPU computing node		<a href="#">Edit</a> <a href="#">Delete</a> <a href="#">Check Condor</a>

# Applications installed

Home > Application		
 Search Application		CREATE/ADD A NEW APPLICATION
Name	Description	Operation
Gromacs	New Text	 Edit  Delete
Amber	Molecular dynamics simulation application used in a variety of simulation programs	 Edit  Delete
CUDA	A parallel computing platform and programming model created by NVIDIA	 Edit  Delete















# Commands installed

Home > Command

 Search Command

CREATE/ADD A NEW COMMAND

String	Description	Pool ID	Application ID	Operation		
/usr/local/cuda-8.0/bin/nvcc	Compilation CUDA	1	3	 Edit	 Delete	 See arguments
/usr/local/gromacs/bin/gmx	Standard Gromacs	1	1	 Edit	 Delete	 See arguments
/usr/bin/mpirun	Running MPI	2	1	 Edit	 Delete	 See arguments
./	Running a Program	1	3	 Edit	 Delete	 See arguments

# Arguments in *Command*

## “/usr/local/gromacs/bin/gmx”









Home > Command > /usr/local/gromacs/bin/gmx			
Search Argument		CREATE/ADD A NEW ARGUMENT	
String	Argument Type	Description	Content Sample
editconf	OTHERS	Config Simualtion Box	-
-f	INPUT	input	conf.gro
-bt	OTHERS	-bt	-
dodecahedron	OTHERS	dodecahedron	-
-o	OUTPUT	output	box.gro
-d	OTHERS	-d	-
0.5	OTHERS	size	-
solvate	OTHERS	Solvating water	-
-cp	INPUT	-cp	box.gro
-p	INPUT	-p	topol.top
mdrun	OTHERS	mdrun	-
-v	OTHERS	-v	-
-deffnm	OTHERS	-deffnm	-
pr	OTHERS	pr	-
-cs	OTHERS	-cs	-
spc216.gro	OTHERS	spc216.gro	-

# Registered users

Home > Users

 Search User

CREATE/ADD A NEW USER

Username	Name	Role	Email	Operation	
admin	admin	admin	admin@admin.com	 Edit	 Delete
ari.w	Ari Wibisono	admin	ari.w@cs.ui.ac.id	 Edit	 Delete
dennis.pratama	Dennis Pratama Kamah	admin	dennis.pratama@ui.ac.id	 Edit	 Delete
heru	Heru Suhartanto	admin	heru@cs.ui.ac.id	 Edit	 Delete

# 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

Successfully adding new experiment  
Lysozyme in Water with ID : 7, and creating  
folder : /home/child1/experiment/7

CLOSE

Name	Description	Folder ID	Application ID	Folder Location	Operation
Gromacs Protein	Gromacs Protein	1	1	/home/child1	<a href="#">Edit</a> <a href="#">Delete</a>

Home >

Search

Successfully Uploading File : 1lyd.pdb

CLOSE

CREATE A FILE

UPLOAD FILES HERE

UPLOADED FILES HERE

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

/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

# Files after submission

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	<a href="#">DOWNLOAD FILE</a>	<a href="#">VIEW FILE</a>
						<a href="#">DELETE FILE</a>	
box.gro	-rw-rw-r--	child1	child1	130114	Des 15, 18:46	<a href="#">DOWNLOAD FILE</a>	<a href="#">VIEW FILE</a>
						<a href="#">DELETE FILE</a>	
conf.gro	-rw-rw-r--	child1	child1	130114	Des 15, 18:45	<a href="#">DOWNLOAD FILE</a>	<a href="#">VIEW FILE</a>
						<a href="#">DELETE FILE</a>	
posre.itp	-rw-rw-r--	child1	child1	40852	Des 15, 18:45	<a href="#">DOWNLOAD FILE</a>	<a href="#">VIEW FILE</a>
						<a href="#">DELETE FILE</a>	
topol.top	-rw-rw-r--	child1	child1	775772	Des 15, 18:45	<a href="#">DOWNLOAD FILE</a>	<a href="#">VIEW FILE</a>
						<a href="#">DELETE FILE</a>	

# 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	<div>Delete</div> <div>Job</div>
/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	<div>Delete</div> <div>Job</div> <div>See Log</div> <div>See Error</div>



# Log of jobs with HTC

Home > Search

Job Name

/usr/local/gro  
editconf -f /ho  
/experiment/7  
/home/child1/  
/7/box.gro -bt

/usr/local/gro  
mdrun -v -deff

000 (043.000.000) 12/15 19:09:00 Job submitted from host: <152.118.31.2  
...  
001 (043.000.000) 12/15 19:09:02 Job executing on host: <152.118.31.20:  
...  
006 (043.000.000) 12/15 19:09:10 Image size of job updated: 568468  
62 - MemoryUsage of job (MB)  
63352 - ResidentSetSize of job (KB)  
...  
006 (043.000.000) 12/15 19:09:26 Image size of job updated: 569224  
62 - MemoryUsage of job (MB)  
63352 - ResidentSetSize of job (KB)  
...  
005 (043.000.000) 12/15 19:09:26 Job terminated.  
(1) Normal termination (return value 0)  
Usr 0 00:01:59, Sys 0 00:00:03 - Run Remote Usage  
Usr 0 00:00:00, Sys 0 00:00:00 - Run Local Usage  
Usr 0 00:01:59, Sys 0 00:00:03 - Total Remote Usage  
Usr 0 00:00:00, Sys 0 00:00:00 - Total Local Usage  
4962 - Run Bytes Sent By Job  
10217591 - Run Bytes Received By Job  
4962 - Total Bytes Sent By Job  
10217591 - Total Bytes Received By Job  
Partitionable Resources : Usage Request Allocated  
Cpus : 1 1  
Disk (KB) : 33347 10000 111600762  
Memory (MB) : 62 1 743  
...

Delete  
b  
Delete  
b  
See Log  
See Error

# Job Output with HTC

```
Home >

:-) GROMACS - gmx mdrun, VERSION 5.1.2 (-:

GROMACS is written by:

Emile Apol      Rossen Apostolov  Herman J.C. Berendsen  Par Bje
Aldert van Buuren  Rudi van Drunen    Anton Feenstra    Sebastian Fri
Gerrit Groenhof  Christoph Junghans  Anca Hamuraru    Vincent Hindr
Dimitrios Karkoulis  Peter Kasson      Jiri Kraus      Carsten Kut
Per Larsson      Justin A. Lemkul    Magnus Lundborg    Pieter Meulen
Erik Marklund      Teemu Murtola      Szilard Pall      Sander Pro
Roland Schulz      Alexey Shvetsov    Michael Shirts     Alfons Sijb
Peter Tieleman     Teemu Virolainen   Christian Wennberg  Maarten Wo

and the project leaders:

Mark Abraham, Berk Hess, Erik Lindahl, and David van der Spoel

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Uppsala University, Stockholm University and
the Royal Institute of Technology, Sweden.
check out http://www.gromacs.org for more information.

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under the terms of the GNU Lesser General Public License
as published by the Free Software Foundation; either version 2.1
of the License, or (at your option) any later version.

GROMACS:      gmx mdrun, VERSION 5.1.2
Executable:    /usr/local/gromacs/bin/gmx
```

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# 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 evenly, 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.