



Cloud Computing Model and Prototype Implementation of Molecular Dynamics Simulations using Amber and Gromacs

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Background Issues

Background Issues

Research Objectives and Benefits

Basis Theory

Research Methodology

Analysis and Discussion

Conclusions and Recommendations

Research Scopes

Computing Resources

Environment Configuration

Application Model

Prototype Development

```
root@riset02:/home/ari# qmgr -c "p s"
#
# Create queues and set their attributes.
#
#
# Create and define queue batch
#
c:
```

The screenshot shows the SCLOUD Cloud Application Manager interface. At the top, there's a header bar with the SCLOUD logo and 'CLOUD APPLICATION MANAGER'. Below it is a navigation bar with 'Login' and 'Register' buttons. The main area is titled 'Member Login:' and contains fields for 'Username:' and 'Password:', each with a corresponding input box. To the right of these fields is a section titled 'Molecular dynamics simulation applications support by SCCloud :'. It lists 'Gromacs' and 'Amber 11', with a note that Gromacs is a versatile package for molecular dynamics and Amber 11 supports parallel simulations. There are links to the 'Gromacs official website' and 'Amber 11 official website'.

```
set server default_queue = batch
set server log_events = 511
set server mail_from = adm
set server scheduler_iteration = 600
set server node_check_rate = 150
set server tcp_timeout = 6
set server mom_job_sync = True
set server keep_completed = 10
set server next_job_number = 158
```

Objectives and Benefits

Background Issues

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Analysis and Discussion

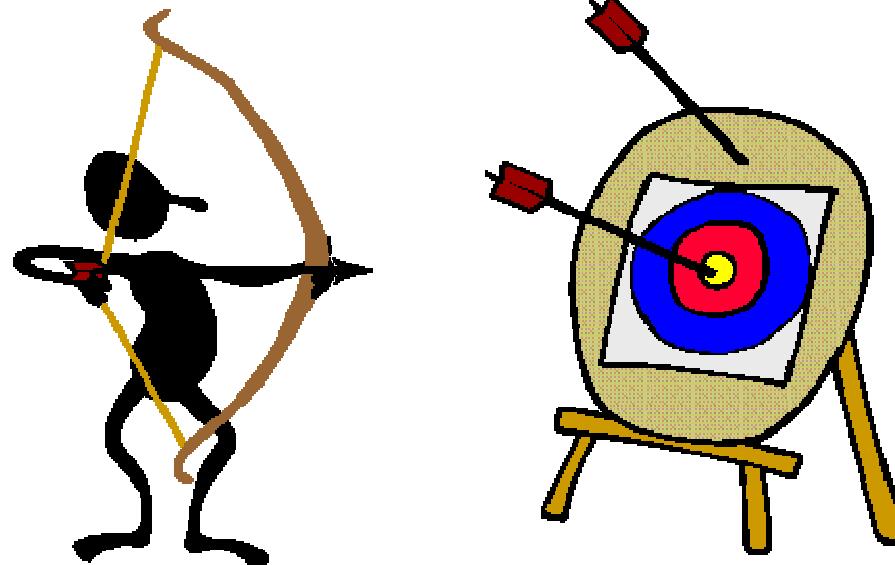
Conclusions

Research Objectives

- Infrastructure Model
- Application Model
- Ease of Access for Molecular Dynamic Simulations

Research Benefit

- Simple Cloud Application
- Basic Understanding of Cloud Application



Source :2)

Molecular Dynamics

Background Issues

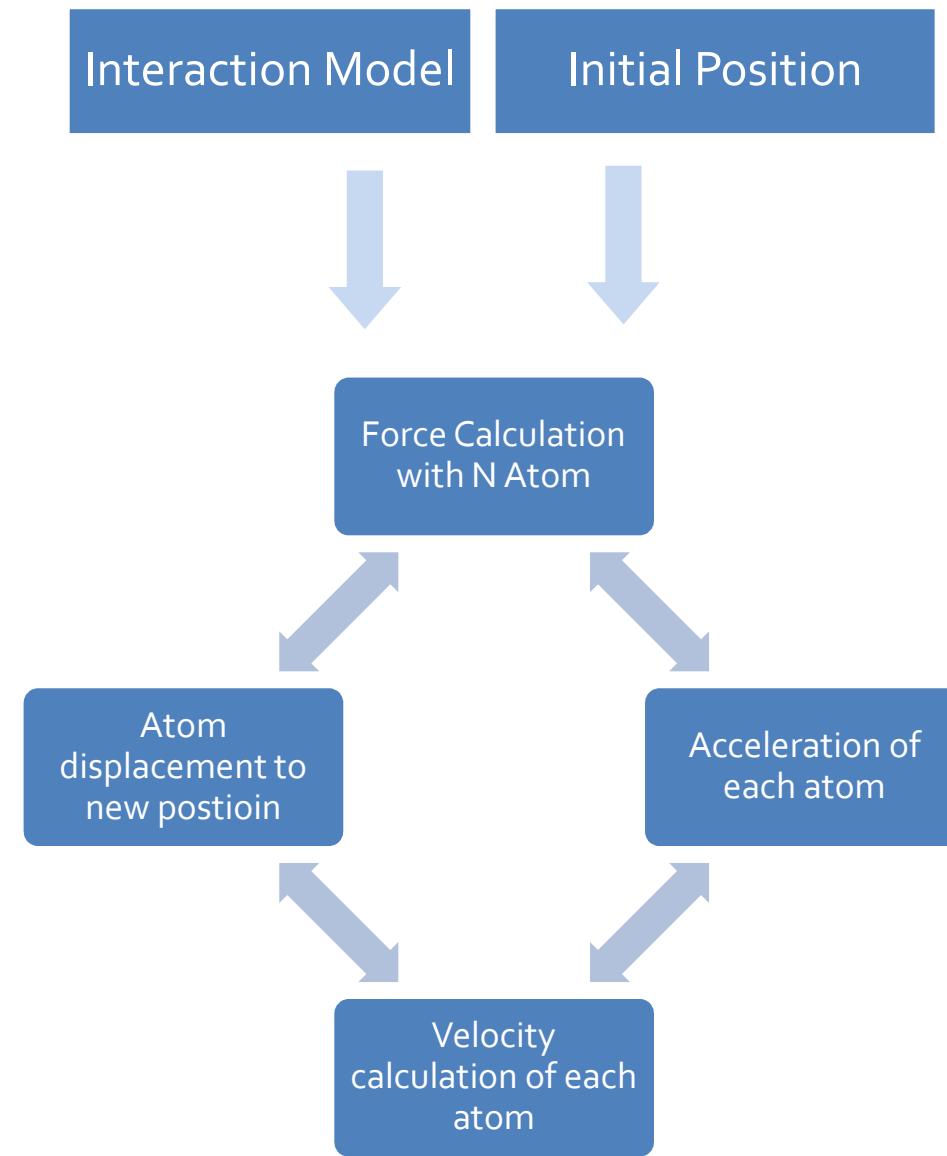
Research Objectives and Benefits

Basis Theory

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Drug Discovery

Background Issues

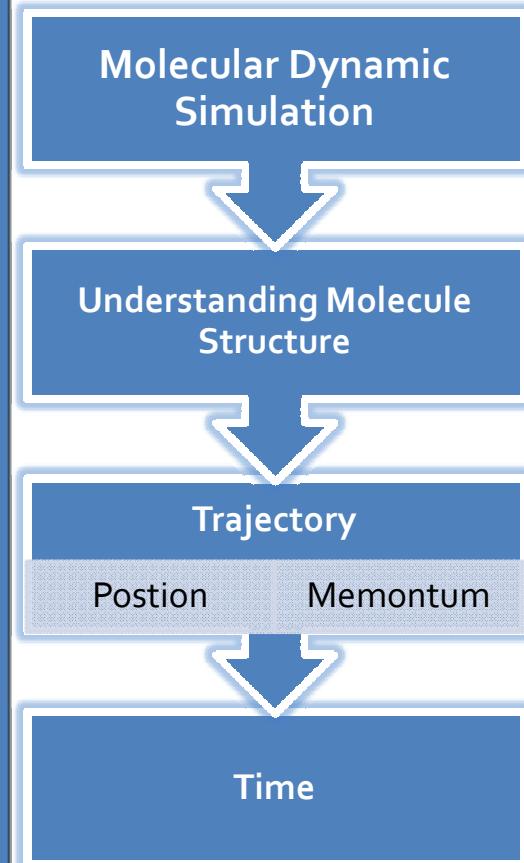
Research Objectives and Benefits

Basis Theory

Research Methodology

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Conclusions



Drug Discovery



Source :9)

Molecular Dynamics Simulations

Background Issues

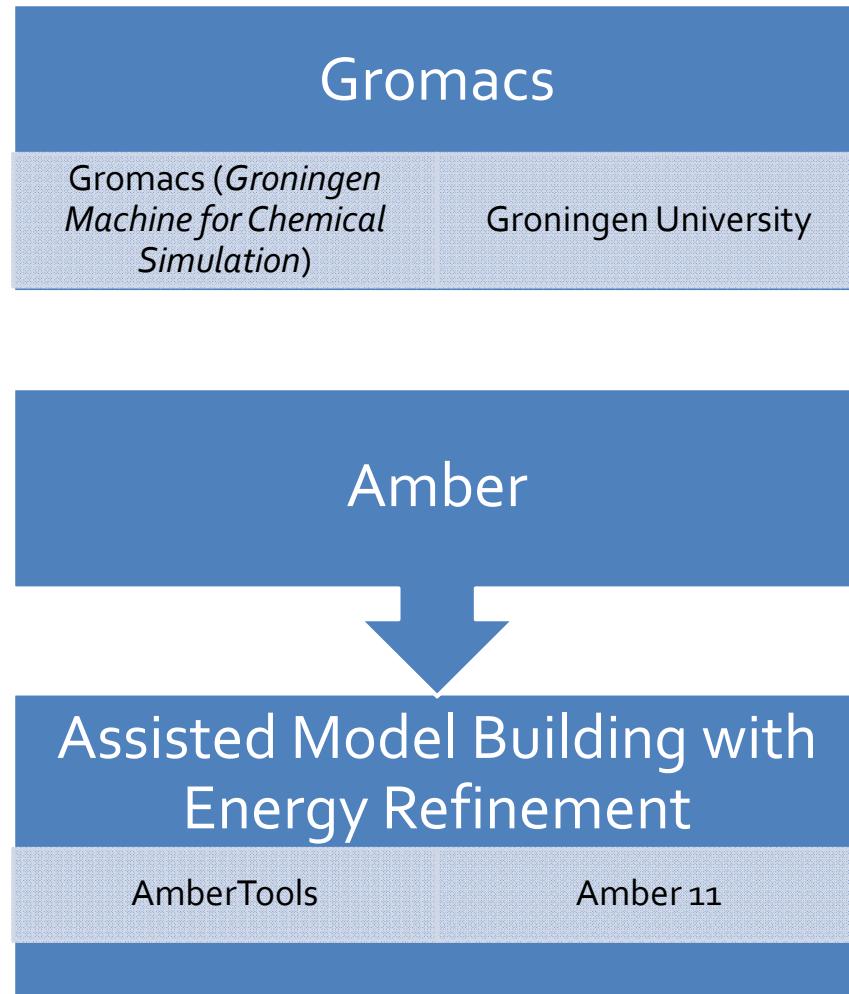
Research Objectives and Benefits

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GROMACS FAST. FLEXIBLE. FREE.



"AMBER is better, it goes up to 11".
(Learn more about real Amber)

Preliminary Study

Background Issues

Research Objectives and Benefits

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Conclusions

Gromacs Simulation

Molecule (Curcumin)

Timestep 1oops - 10oops

1 – 5 Processors

No	timestep	Execution Time Using n processor				
		1	2	3	4	5
1	2oops	13h:37m:38s	7h:23m:47s	5h:32m:34s	4h:26m:20s	3h:38m:48s
2	4oops	1d:03h10m:06s	14h:44m:02s	11h:01m:38s	8h:41m:15s	7h:16m:42s
3	6oops	1d:16h:22m:34s	22h:04m:25s	16h:40m:14s	13h:17m:38s	10h:55m:54s
4	8oops	2d:06h:52m:48s	1d:03h:02:m46s	22h:11m:54s	17h:46m:35s	14h:35m:29s
5	10oops	2d:21h:22m:57	1d:13h:00m:25s	1d:03h:41m:49s	22h:06m:03s	18h:09m:47s

Preliminary Study

Background Issues

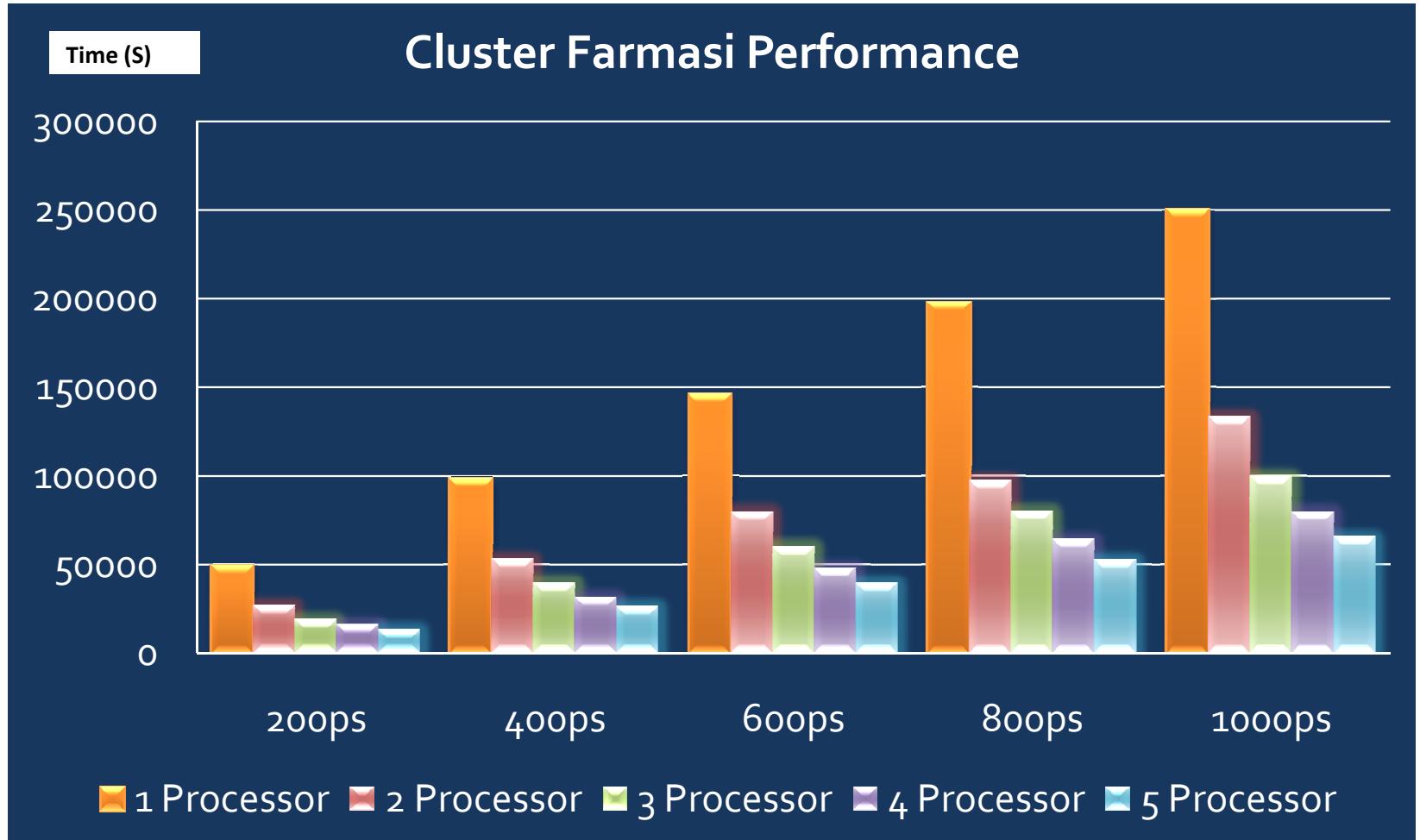
Research Objectives and Benefits

Basis Theory

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Conclusions



Preliminary Study

Background Issues

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Amber Simulation

Molecule (Curcumin)

Timestep 1oops - 4oops

1,2,4,8 Processors

timestep	Simulation time based on the number of processors			
	1	2	4	8
100	1h :48m	1h:1m	54m	24 m
200	3h:42m	2hr	1h:15m	48 m
300	5h:36m	3h:12m	1h:54m	1h:18m
400	7h:30m	4h:9m	2h:30m	1h:36m

Cloud Computing Concept

Background Issues

Research Objectives and Benefits

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Conclusions a

Cloud Model

Cloud Characteristics

on-Demand selfservice

Broad Network Access

Resource Pooling

Rapid Elasticity

Measured Service

Cloud Service Model

Software As A Service

Platform As A Service

Infrastructure As A Service

Cloud Deployment Model

Public Cloud

Private Cloud

Community Cloud

Hybrid Cloud

Research Methodology

Background Issues

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Conclusions

Literature Study

- Application Manual
- Cloud Theory

Infrastructure Preparation

- Network Design
- Computing Resources Setup

Software Installation

- OS Installation
- Software Installation

Modeling Cloud Application

- Requirement Gathering
- Designing Cloud Application

Model Implementation

- Develop Application Prototype

Evaluation

- Simulation Testing
- User Acceptance Test

Source :3

Hardware Specifications

Background Issues

Research Objectives and Benefits

Basis Theory

Research Methodology

Analysis and Discussion

Conclusions



Hardware (4 Buah Computing Node)

- Intel Quad Core, 2.8GHz, 8MB Cache
- RAM 2x 2GB, DDR3, PC-12800
- Motherboard Gigabyte
- Power Supply 750 W,
- Internal DVD-RW, SATA
- HDD 640GB, 7200RPM, SATA II
- NVIDIA GeForce GTX 465 (1 buah), NVIDIA GeForce GTX 470 (2 buah), NVIDIA Quaddro 4000 (1 buah)

Hardware (1 Buah Web Application Server)

- Core 2 Duo, 2.8GHz, 8MB Cache
- 2GB, DDR3, PC-12800
- Motherboard Asus
- Power Supply 450W
- Internal DVD-RW, SATA
- HDD 120 GB, 7200RPM,
- NVIDIA GeForce GTS 250

Network Design

Background Issues

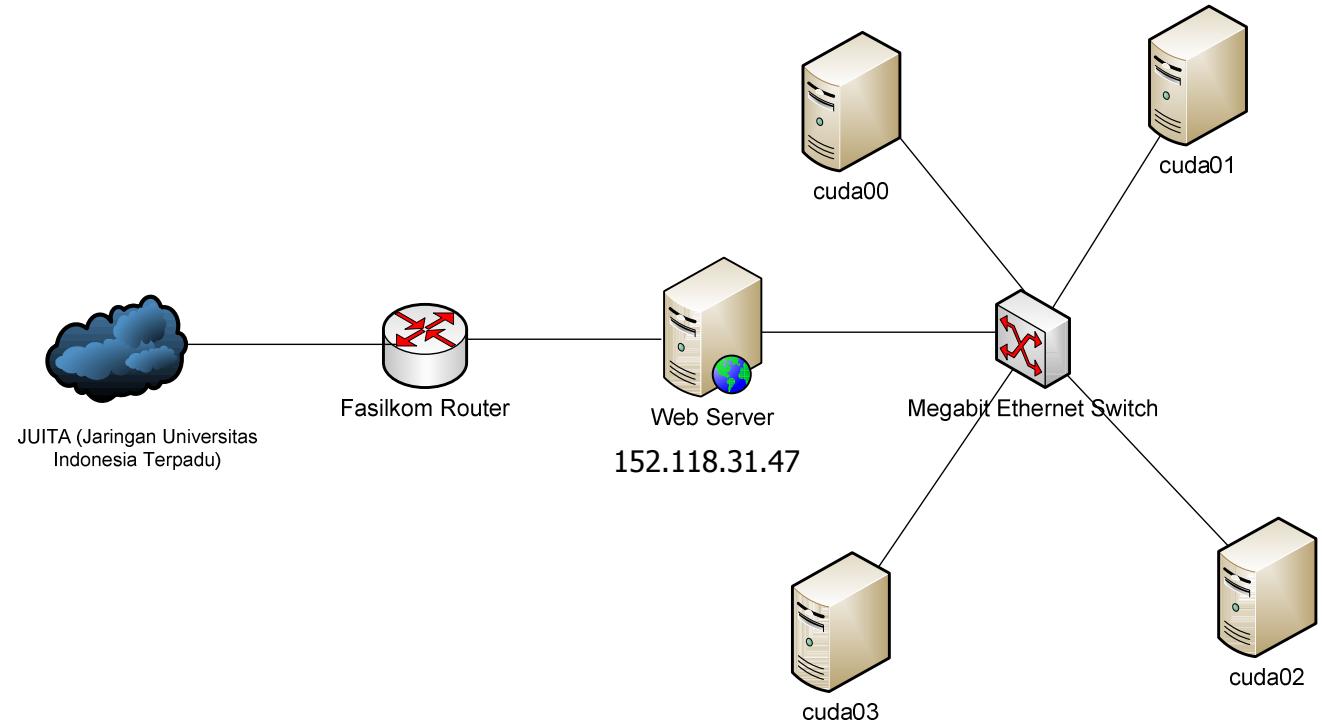
Research Objectives and Benefits

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Software Installation

Background Issues

Research Objectives and Benefits

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Conclusions

Web Application Server OS: Ubuntu 10.04

Supporting Application

- XAMPP 1.7.7 for Linux
- PBS Job Scheduler



Computing Node (OS): Ubuntu 10.04

Supporting Application

- MPI (Message Passing Interface)
- PBS Job Scheduler

Main Application

- Gromacs 4.5.3
- Amber 11

GROMACS
FAST.
FLEXIBLE.
FREE.

Amber Home Page

"AMBER is better, it *goes up to 11*".
(Learn more about real Amber)

Application Design

Background Issues

Research Objectives and Benefits

Basis Theory

Research Methodology

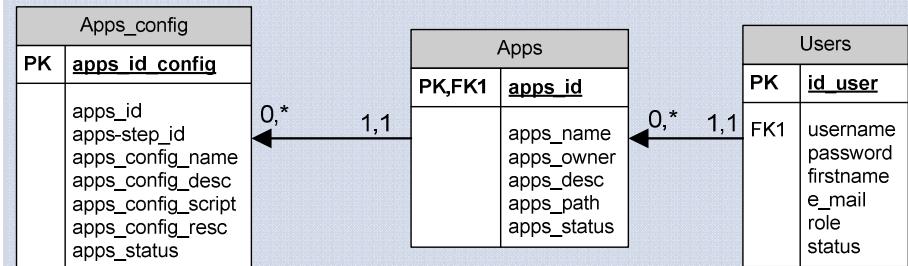
Analysis and Discussion

Conclusions and Recommendations

Fitur

- *Login*
- *User Registration*
- *Edit User Data*
- *View User Information*
- *View Application*
- *Create Application*
- *Delete Application*
- *Create Application Configuration*
- *Add Application Configuration*
- *Delete Application Configuration*
- *Edit Application Configurations*
- *Run Application*
- *Manage Data*
- *Simulation Execution*
- *View execution status*
- *Manage Jobs Scheduler*
- *Manage User*

Database Design



SCLOUD

CLOUD APPLICATION MANAGER

Login Register

Member Login :

Username :

arizbw

Password :

Login

Molecular dynamics simulation applications support by SCCloud :

Gromacs

GROMACS is a versatile package to perform molecular dynamics, it is primarily designed for biochemical molecules like proteins, lipids and nucleic acids that have a lot of complicated bonded interaction. SCCloud web interface equipped with gromacs 4.5.3 and MPI support to perform parallel molecular dynamic simulations. Further details about Gromacs Application can be found in the [Gromacs official website](#).

Amber 11

Amber is the collective name for a suite of programs that allow users to carry out molecular dynamics simulations, particularly on biomolecules. SCCloud web interface assembled with Amber 11 and equipped with MPI support to do parallel molecular modeling simulation. The brief explanation about Amber Application can be found in [this link](#).

Application Model

Background Issues

Research Objectives and Benefits

Basis Theory

Research Methodology

Analysis and Discussion

Conclusions

Cloud Characteristics

On Demand Self-service
• Configuration
• Computing Resources

Broad Network Access

Resource Pooling

Rapid Elasticity

Measured Service

User Management Application Management Logout

Application Configuration

Step 1 Configuration

Step 1 name Step 1 number of available resources
1 node

Step 1 script Step 1 Description

Add step Remove Add Save Data

Step 1 number of available resources

1 node

1 node
2 node
3 node
4 node
5 node
6 node
7 node
8 node
9 node
10 node
11 node
12 node
13 node
14 node
15 node
16 node

Sccloud Application Model

Background Issues

Research Objectives and Benefits

Basis Theory

Research Methodology

Analysis and Discussion

Conclusions

Cloud Characteristics

On Demand Self-service

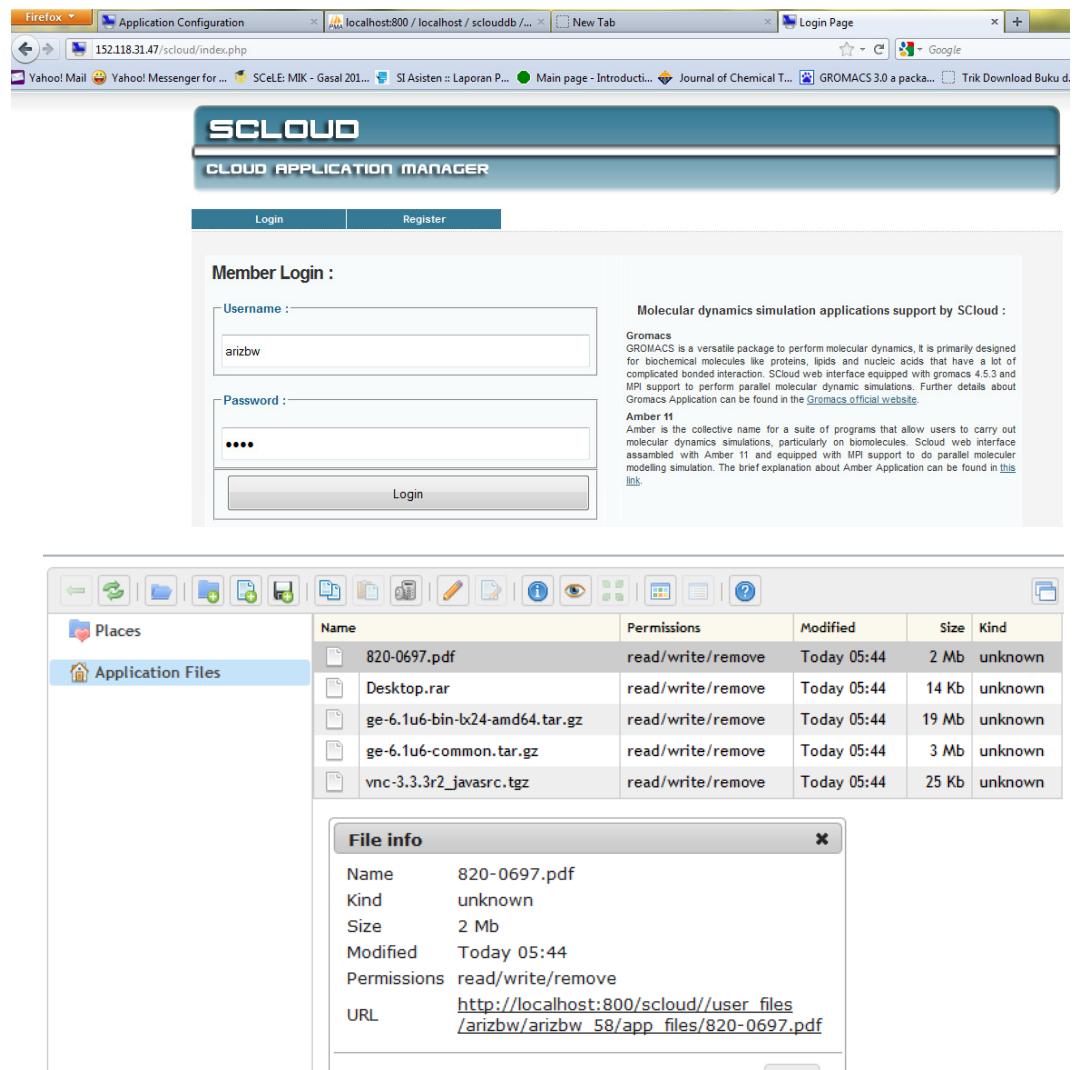
- Configuration
- Computing Resources

Broad Network Access

Resource Pooling

Rapid Elasticity

Measured Service



Application Model

Background Issues

Research Objectives and Benefits

Basis Theory

Research Methodology

Analysis and Discussion

Conclusions

Cloud Characteristics

On Demand Self-service

- Configuration
- Computing Resources

Broad Network Access

Resource Pooling

Rapid Elasticity

Measured Service

Computing Resources



Scloud Application Model

Background Issues

Research Objectives and Benefits

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Cloud Characteristics

On Demand Self-service

- Configuration
- Computing Resources

Broad Network Access

Resource Pooling

Rapid Elasticity

Measured Service

User Management	Job Management	Logout
Job Management Information		
Job Machine Id	Step Name	Runtime
152.riset02	grom_simms	72:41:00
153.riset02	grom10ps	0
154.riset02	grom20ps	0
155.riset02	Gromac30ps	0
156.riset02	grom40ps	0
157.riset02	grom50ps	0

Status
Running
Queuing

How Scloud Work?

Background Issues

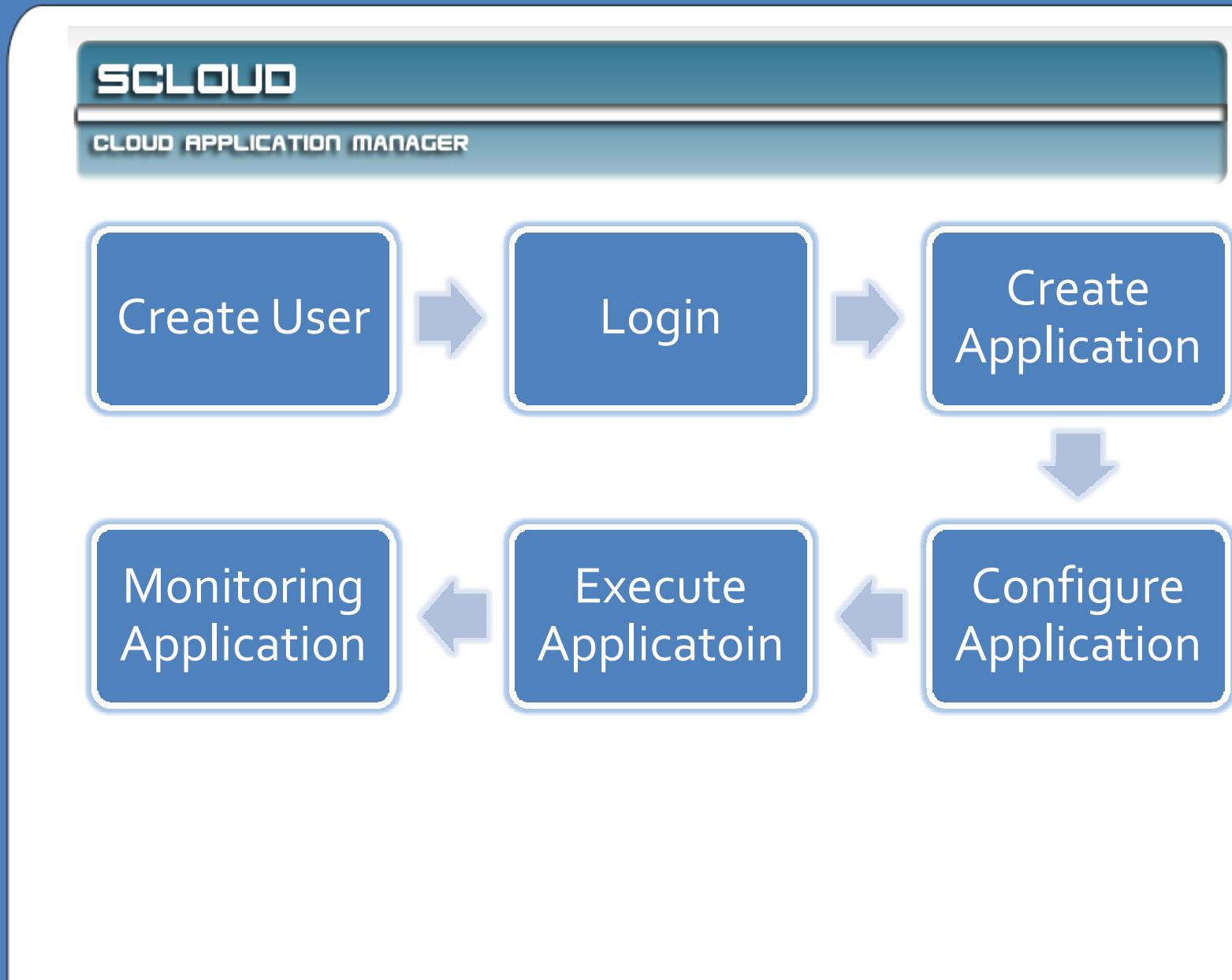
Research Objectives and Benefits

Basis Theory

Research Methodology

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Conclusions





Create user -> Authenticate User -> User Login

Firefox Login Page 152.118.31.47/scloud/index.php Google Bookmarks

Yahoo! Mail Yahoo! Messenger for ... SCeLE: MIK - Gasal 201... SI Asisten :: Laporan P... Main page - Introducti... Journal of Chemical T... GROMACS 3.0 a packa... Trik Download Buku d... Bookmarks

SCLOUD
CLOUD APPLICATION MANAGER

Login Register

Member Login :

Username : * Please fill out this field

Password :

Molecular dynamics simulation applications support by SCCloud :

Gromacs
GROMACS is a versatile package to perform molecular dynamics, It is primarily designed for biochemical molecules like proteins, lipids and nucleic acids that have a lot of complicated bonded interaction. SCcloud web interface equipped with gromacs 4.5.3 and MPI support to perform parallel molecular dynamic simulations. Further details about Gromacs Application can be found in the [Gromacs official website](#).

Amber 11
Amber is the collective name for a suite of programs that allow users to carry out molecular dynamics simulations, particularly on biomolecules. SCcloud web interface assembled with Amber 11 and equipped with MPI support to do parallel molecular modelling simulation. The brief explanation about Amber Application can be found in [this link](#).



sCLOUD
CLOUD APPLICATION MANAGER

User Management Application Management Logout

Sccloud Application Management

Apps ID	Application Name	Application Owner	Application Status	Delete	Execute
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arizbw, Application and Design: - [sCloud](#)

C:\...\Desktop\app_files

Name	Ext
..	
md.gro	
md_50ps.mdp	
Prot.top	

.../mirror/htdocs/scloud/user_files/ari.wibisor

Name	Ext
..	

0 B of 412 KB in 0 of 3 0 B of 0 B in 0 of 0

F2 Rename F4 Edit F5 Copy F6 Move F7 Create Director

This screenshot shows the sCloud Cloud Application Manager. The interface includes a header with the sCloud logo and "CLOUD APPLICATION MANAGER". Below the header is a navigation bar with "User Management", "Application Management" (which is currently selected), and "Logout". The main content area is titled "Sccloud Application Management". At the bottom of the main area, there is a copyright notice: "arizbw, Application and Design: - [sCloud](#)". To the right of the main content are two file explorer windows. The left window shows files in the directory "C:\...\Desktop\app_files", including "md.gro", "md_50ps.mdp", and "Prot.top". The right window shows files in the directory ".../mirror/htdocs/scloud/user_files/ari.wibisor", which is currently empty. Both file explorers include standard file operations like Rename, Edit, Copy, Move, and Create Director.



sCloud

CLOUD APPLICATION MANAGER

User Management Application Management Logout

Scloud Application Management

Apps ID	Application Name	Application Owner	Application Status	Delete	Execute
173	groms 50 ps	ari.wibisono	Configure Now	Delete	Execute Apps

arizbw, Application and Design: - sCloud

C:\...\Desktop\app_files /.../user_files/ari.wibisono/ari.wibisono_173

Name	Ext
..	
md.gro	
md_50ps.mdp	
Prot.top	

Name	Ext
..	
app_files	

0 B of 412 KB in 0 of 3 0 B of 0 B in 0 of 1

F2 Rename F4 Edit F5 Copy F6 Move F7 Create Directory



Execute Application (Step 6)

Background Issues

Research Objectives and Benefits

Basis Theory

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Conclusions and Recommendations

SCLOUD

CLOUD APPLICATION MANAGER

User Management Application Management Logout

Sccloud Application Management

Apps ID	Application Name	Application Owner	Application Status	Delete	Execute
173	groms 50 ps	ari.wibisono	Configured	Delete	Execute Apps

arizbw,



Execute Application (Step 1) -> Monitoring Application

Background Issues

Research Objectives and Benefits

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SCLOUD
CLOUD APPLICATION MANAGER

Application Management

Application groms 50 ps

File Manager

Step 0 **Step 1**

<p>Step Name : <input type="text" value="grom_prep"/></p> <p>Step Resources : <input type="text" value="1 node"/></p>	<p>Step Description : <input type="text" value="Preparation Gromacs 50ps"/></p> <p>Step Execution Script : <input type="text" value="\$gromacs/grompp -f \$home/md_50ps.mdp -c \$home/md.gro -p \$home/Prot.top -o \$home/md_50ps.tpr"/></p>	<p>Home Folder Files (Drag and drop the filename to script execution textarea)</p> <p>Configuration Settings: \$home \$resources \$machinefile \$gromacs \$amber</p> <p>User Files: \$home/md_50ps.mdp \$home/grom_prep.o142 \$home/md_50ps.tpr \$home/grom_prep.e142 \$home/.tmb \$home/md.gro \$home/ari.wibisono_173_0.sh \$home/Prot.top</p>
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Cloud Application Evaluation

Background Issues

Research Objectives and Benefits

Basis Theory

Research Methodology

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Conclusions and Recommendations

Self Experiment

- Protein Simulation
- Timestep 10ps -50ps
- Resources 16 Processor

User Acceptance Test

- Protein Simulation
- Timestep 50ps
- Resources 8 Processor

User Management Job Management Logout

Job Management Information

Job Machine Id	Step Name	Runtime	Status	Job Deletion
152.riset02	grom_simms	72:41:00	Running	Delete Job
153.riset02	grom10ps	0	Queuing	Delete Job
154.riset02	grom20ps	0	Queuing	Delete Job
155.riset02	Gromac30ps	0	Queuing	Delete Job
156.riset02	grom40ps	0	Queuing	Delete Job
157.riset02	grom50ps	0	Queuing	Delete Job

Self Experiment Result..1 (gromacs)

Background Issues

Research Objectives and Benefits

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Preparation Script

```
input file : md_10psmdp, Prot.top, md.gro  
output file : md_10ps.trr
```

```
/home/ari/mirror/Programs/gromacs45/bin/grompp -f  
/home/ari/mirror/simulasi_tesis_2011/wibisono_65/md_10ps.mdp -p  
/home/ari/mirror/simulasi_tesis_2011/wibisono_65/Prot.top -c  
/home/ari/mirror/simulasi_tesis_2011/wibisono_65/md.gro -o  
/home/ari/mirror/simulasi_tesis_2011/wibisono_65/md_10ps.tpr
```

Simulation Script

```
input file : md_10psmdp, Prot.top, md.gro  
output file : md_10ps.trr
```

```
mpirun -np 16 -machinefile /home/ari/mirror/mpd.hosts  
/home/ari/mirror/Programs/gromacs45/bin/mpi_mdrun -s  
/home/ari/mirror/simulation_tesis_2011/wibisono_65/md_10ps.tpr -o  
/home/ari/mirror/simulation_tesis_2011/wibisono_65/md_prod_10ps.trr  
-c /home/ari/mirror/simulation_tesis_2011/wibisono_65/md.gro
```

Self Experiment Result..2 (gromacs)

Background Issues

Research Objectives and Benefits

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Step Number	Step Name	Output Size (Manual)	Output Size (Scloud)
Gromacs 10ps			
0	Gromacs 10ps Preparation	0.19 MB	0.19 MB
	Resource : 1 Processor		
1	Gromacs 10ps Simulation	11.7 MB	11.7 MB
	Resource : 16 Processor		
Gromacs 20ps			
0	Gromacs 20ps Preparation	0.19 MB	0.19 MB
	Resource : 1 Processor		
1	Gromacs 20ps Simulation	23.4 MB	23.4 MB
	Resource : 16 Processor		
Gromacs 30ps			
0	Gromacs 30ps Preparation	0.19 MB	0.19 MB
	Resource : 1 Processor		
1	Gromacs 30ps Simulation	35.1 MB	35.1 MB
	Resource : 16 Processor		
Gromacs 40ps			
0	Gromacs 40ps Preparation	0.19 MB	0.19 MB
	Resource : 1 Processor		
1	Gromacs 40ps Simulation	46.7 MB	46.7 MB
	Resource : 16 Processor		
Gromacs 50ps			
0	Gromacs 50ps Preparation	0.19 MB	0.19 MB
	Resource : 1 Processor		
1	Gromacs 50ps Simulation	58.4 MB	58.4 MB
	Resource : 16 Processor		

Self Experiment Result..1 (amber)

Background Issues

Research Objectives and Benefits

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Simulation Script

```
input file : rad_vac_gb0_md1_12Acut_20ps.in, rad_vac_gb0_gb1.prmtop,  
rad_vac_gb0_init_min.rst  
  
output file : rad_vac_gb0_md1_12Acut_20ps.out, rad_vac_gb0_md1_12Acut_20ps,  
rad_vac_gb0_md1_12Acut_20ps.mdcrd
```

```
mpirun -np 16 -machinefile /home/ari/mirror/mpd.hosts  
/home/ari/mirror/Programs/amber11/exe/sander.MPI -O -i  
/home/ari/mirror/simulation_tesis_2011/wibisono_72/rad_vac_gb0_md1_12Acut_20ps.in -o  
/home/ari/mirror/simulation_tesis_2011/wibisono_72/rad_vac_gb0_md1_12Acut_20ps.out -p  
/home/ari/mirror/simulation_tesis_2011/wibisono_72/rad_vac_gb0_gb1.prmtop -c  
/home/ari/mirror/simulation_tesis_2011/wibisono_72/rad_vac_gb0_init_min.rst -r  
/home/ari/mirror/simulation_tesis_2011/wibisono_72/rad_vac_gb0_md1_12Acut_20ps.rst -x  
/home/ari/mirror/simulation_tesis_2011/wibisono_72/rad_vac_gb0_md1_12Acut_20ps.mdcrd
```

Self Experiment Result..2 (amber)

Background Issues

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No	Step Name	Output Size (Manual)	Output Size (Scloud)
1 Amber 1ops			
	Amber 1ops Simulation	0.02 MB	0.02 MB
	Resource : 16 Processor	0.6 MB	0.6 MB
		0.1 MB	0.1 MB
2 Amber 2ops			
	Amber 2ops Simulation	0.02 MB	0.02 MB
	Resource : 16 Processor	1.2 MB	1.2 MB
		0.1 MB	0.1 MB
3 Amber 3ops			
	Amber 3ops Simulation	0.02 MB	0.02 MB
	Resource : 16 Processor	1.8 MB	1.8 MB
		0.1 MB	0.1 MB
4 Amber 4ops			
	Amber 4ops Simulation	0.02 MB	0.02 MB
	Resource : 16 Processor	2.4 MB	2.4 MB
		0.1 MB	0.1 MB
4 Amber 5ops			
	Amber 5ops Simulation	0.02 MB	0.02 MB
	Resource : 16 Processor	3.1 MB	3.1 MB
		0.1 MB	0.1 MB

User Acceptance Test

Background Issues

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User Acceptance Test

- Protein Simulation
- Gromacs + Amber
- Timestep : 50ps
- Resources : 8 Processor
- 8 UAT

S/No.	Action	Expected Results	Actual Results	Waktu Pengoperasian Fitur	Level Kesalahan	Level Kemudahan	Level Kepuasan	Saran
		E.G Berhasil atau tidak	E.G Berhasil atau tidak	E.G 1 Jam atau 20 Menit atau 5 detik	E.G 1 , 6, 7 (input Integer)	E.G 1, 2, 3, 4, 5, 6 (select from drop down list)	E.G 1, 2, 3, 4, 5, 6 (select from drop down list)	E.G Sistem navigasinya masih perlu diperbaiki
UseCase #01: Login								
1.1	Membuka halaman aplikasi scloud	Menampilkan halaman berbentuk form berisi username, dan pasword	berhasil					
1.2	Mengisi username, password	Sistem melakukan verifikasi data-data yang diisi. Jika proses login berhasil maka sistem akan me-redirect ke dalam page User Information (Sesuai dengan rolenya masing-masing)	berhasil	2 menit		1 6 (Sangat Mudah)	4 (Cukup Puas)	sudah cukup baik

User Acceptance Test

Background
Issues

Research
Objectives and
Benefits

Basis Theory

Research
Methodology

*Analysis and
Discussion*

Conclusions

No	Parameter	Evaluation Test
1	Feature Operation	100 %
2	The average duration of utilization of all the features from start to finish	2206 detik atau kurang lebih 36.7 menit
3	Average Errors made by user	2 x times each features

Conclusions

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Conclusions

- The successful development of simple application using the cloud computing concept
- Giving the Customized Configuration Application, Resource On-Demand Application, File management based on user preferences
- Makes it easy for users of molecular dynamics simulations to run simulations easily

Background
Issues

Research
Objectives and
Benefits

Basis Theory

Research
Methodology

Analysis and
Discussion

Conclusions



References

Latar Belakang
Permasalahan

Tujuan dan
Manfaat
Penelitian

Landasan Teori

Metodologi
Penelitian

Analisis dan
Pembahasan

**Kesimpulan dan
Saran**

1. http://2.bp.blogspot.com/_hwc-QMwo1iY/St64X9xmklI/AAAAAAAACHs/E5GgOjAcTrw/s400/question-mark1a.jpg
2. <http://joseroyhipolito.files.wordpress.com/2011/02/purpose.gif>
3. http://sixthsense.osfc.ac.uk/chemistry/atomic_structure2/atom.gif
4. <http://bikeadvice.s3.amazonaws.com/wp-content/uploads/2009/02/water.jpg>
5. <http://www.dicts.info/img/ud/protein.jpg>
6. <http://www.polyplus-transfection.com/wp-content/uploads/2009/08/invivo-jetPEI-fig4.jpg>
7. <http://www.lifesitenews.com/ldn/images/2006/ln%20vitro.jpg>
8. http://blogs.guardian.co.uk/technology/archives/images/hp_mediasmart_whs.jpg
9. <http://1.1.1.1/bmi/www.dagraphic.com/images/catalogselect/catalogNVIDIA.jpg>
10. http://to.gstatic.com/images?q=tbn: vUwu4hE7kypRM::&t=1&usq=_5zpbp2w6G2S22k_Tqp5ME87ChjA=