

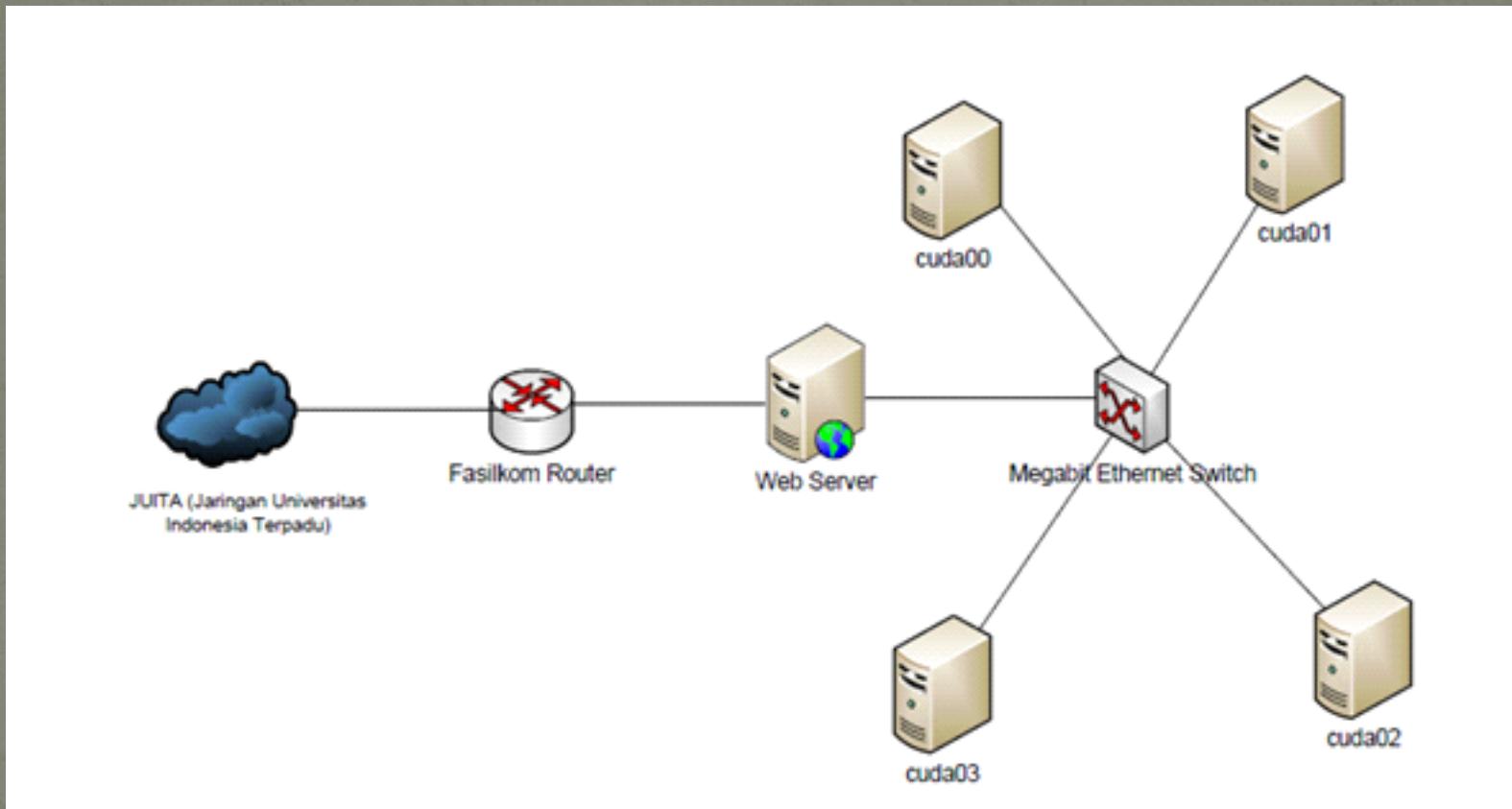
Autodock Application Integration into SCLOUD Web Interface

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Introduction

- Cloud Computing is a solution
- Because it can utilize computational methods in accordance with the needs of the user application.
 - eg. Dynamic Molecular
- SCLOUD, an application-based cloud application that assist simulation such as Amber, Gromacs and Autodock

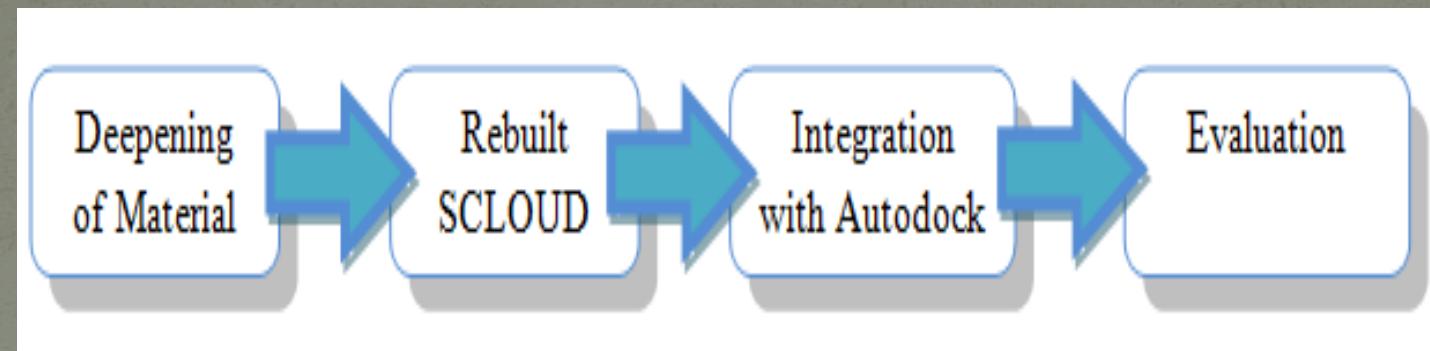
Scloud Topologi



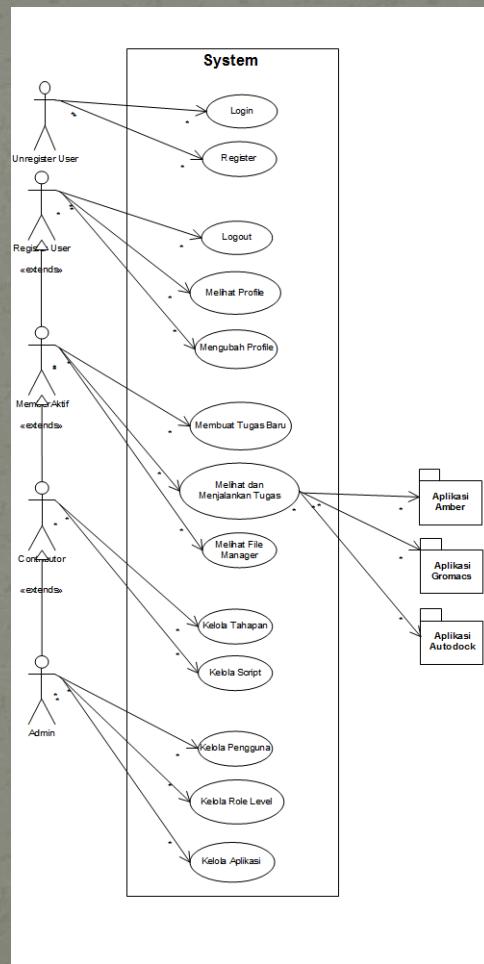
Materials and methods

- Four iterable process
 - Deepening Material
 - Study Literatur
 - Remake SCLOUD using Yii framework.
 - Integration to Autodock Vina
 - Evaluation
 - performance evaluation
 - needs evaluation
 - user evaluation
 - expert evaluation.
- SCLOUD will build in and using:
 - OS, Ubuntu 12.04 LTS.
 - NFS
 - OpenMPI
 - Torque (PBS Scheduler)
 - Gromacs, Amber, dan Autodock Vina.
 - Web Server Software.

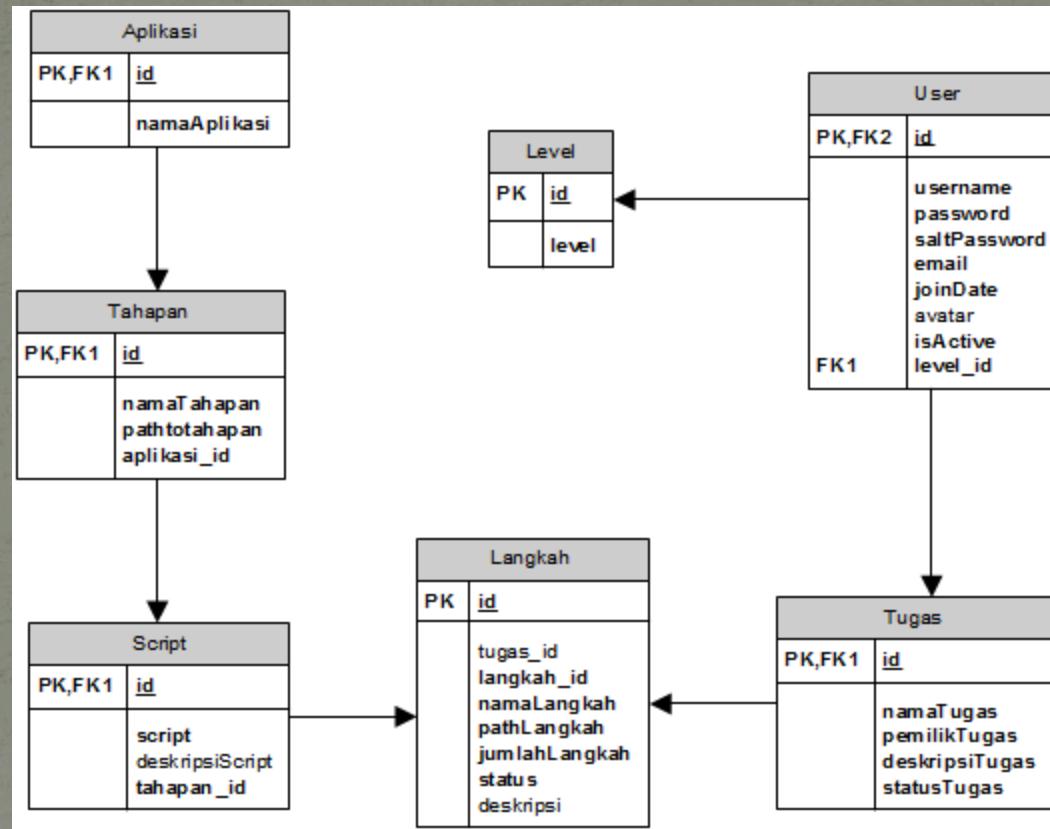
Research Methodology



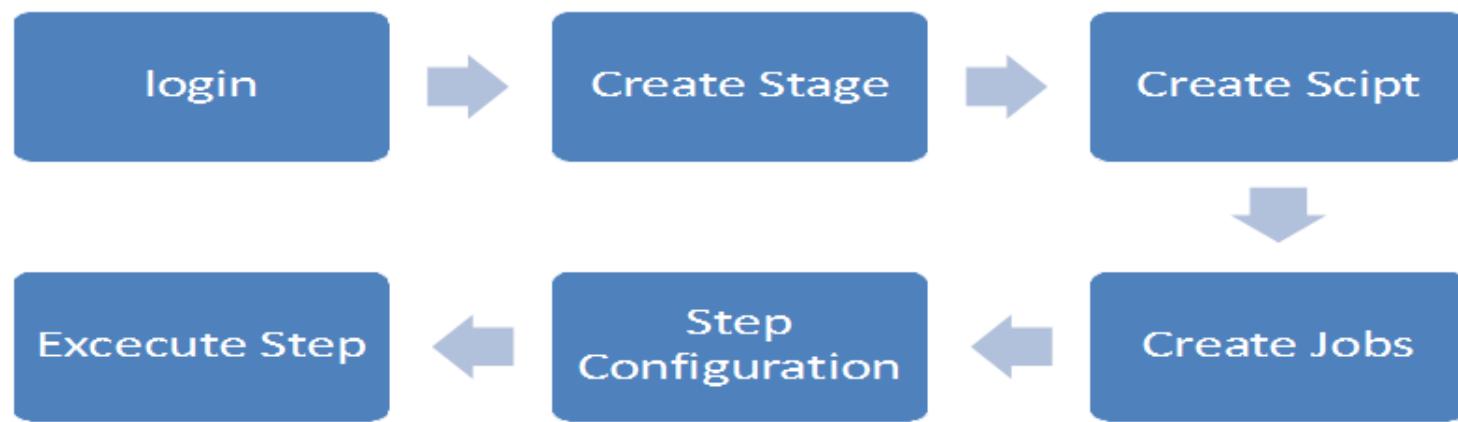
Use Case SCLOUD



SCLOUD Database Structure



SCLLOUD Process State



Running Vina Via SCLOUD

View Tugas #25

ID	25
Nama Tugas	Autodock Vina
Pemilik Tugas	scloud
Deskripsi Tugas	Autodock Vina
Status Tugas	new
Proses	Execute All

View Langkah #0

ID	45
Deskripsi	Memasukkan ligands dan receptor dalam bentuk file zip
script	* #LIGANDZIP #RECEPTORZIP
Status	COMPLETE
Execute	Execute
Konfigurasi	Konfigurasi

View Langkah #1

ID	46
Deskripsi	Menjalankan Autodock Vina
script	* #fileconfig ?
Status	COMPLETE
Execute	Execute
Konfigurasi	Konfigurasi

Evaluation

No	Parameter	Nilai
1	Pengoperasian Fitur	100% berhasil
2	Rata – rata Waktu Pengoperasi an Fitur	4.41 detik
3	Rata – rata Kesalahan	0.4 x, jarang sekali terjadi kesalahan
4	Rata –rata Level Kemudahan	5.28 (Mudah)
5	Rata – rata Level Kepuasan	5.26 (Puas)

Conclusions

- SCLOUD expected to contribute in the field of molecular dynamics.
- SCLOUD application development is done two things:
 - remake SCLOUD with Yii framework
 - integrate Autodock vina features on the system.
- SCLOUD application users are permitted to
 - perform molecular dynamics simulations.
 - given the opportunity to choose the configuration that has been set by an expert so do not need to search for the configuration to be used.
- Expected by using this application, the use and development in the field of molecular dynamics can be easily done.

Thank you
