

# **THE CURRENT STATUS OF MGRID**

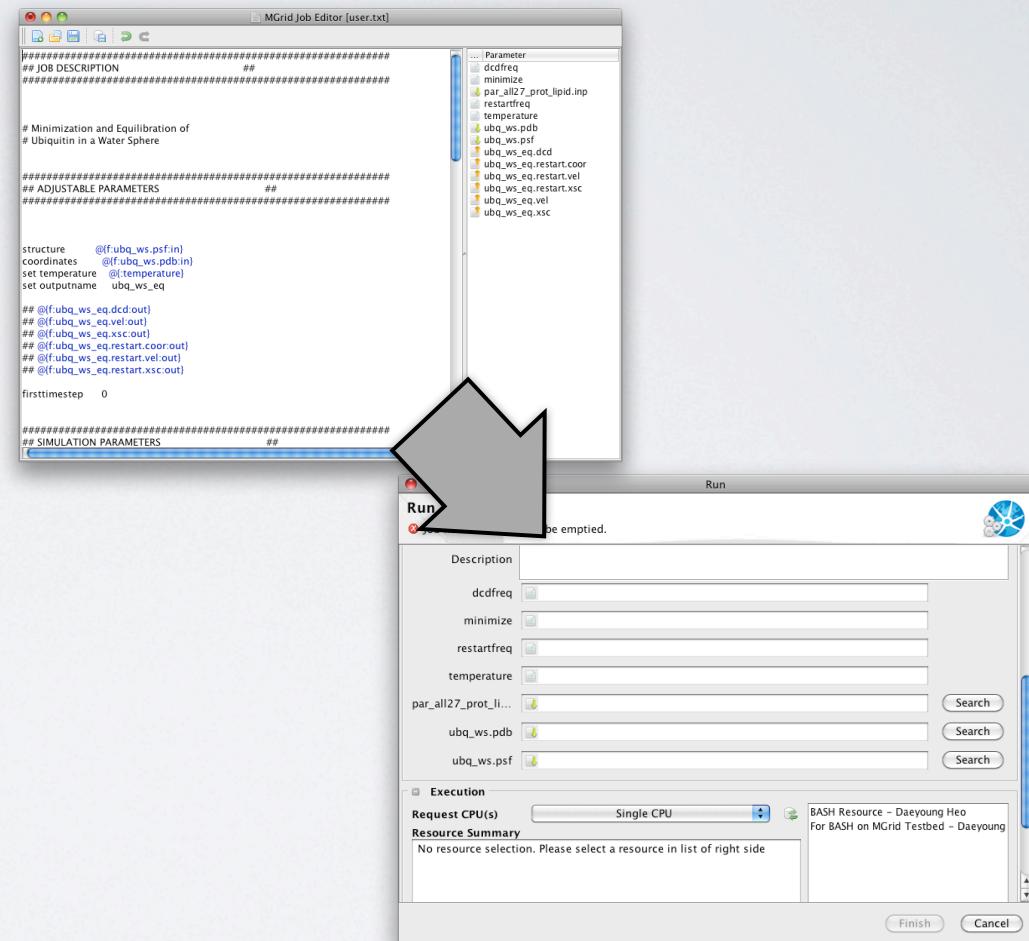
*INTEGRATE WITH GFARM,  
LEGACY TOOLS AND SNS*

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- Reduced number of steps for Job Execution
- Support gfarm exploring.
- Convenient way of sign-in.
- Let legacy desktop tools to access simulation data as if regular file on local storage
- Programmable parameter sweeping for bulk simulation.
- Integragte SNS for sharing: support blog.

# REDUCE #STEPS FOR JOB EXECUTION

- 7 steps >> 2 steps.
- Form Autocompletion



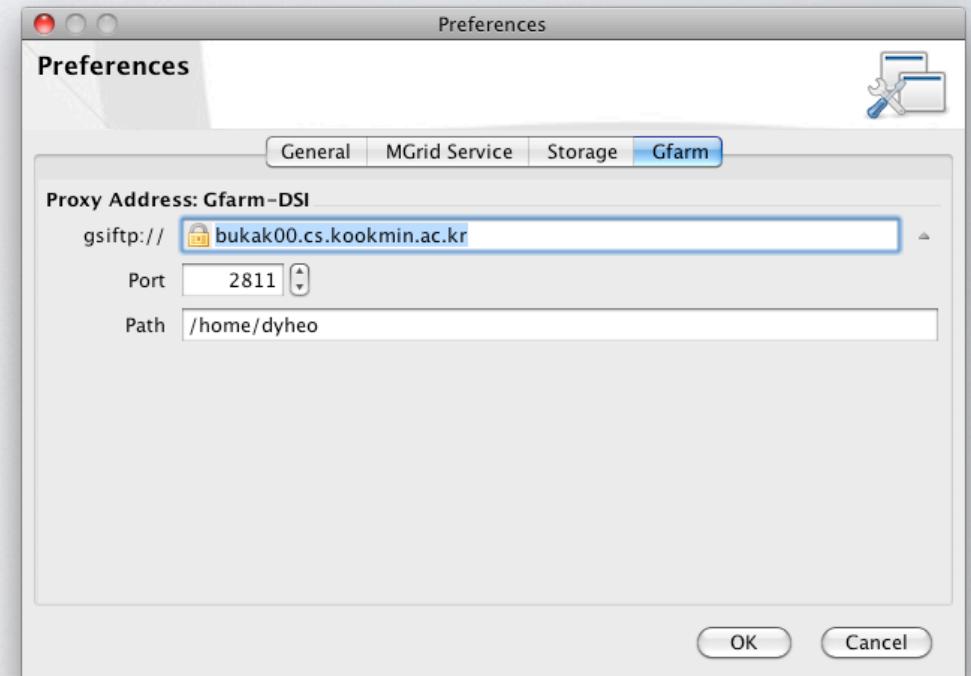


# MGrid Tutorial D

How to do simulation  
on the MGrid System?

# GFARM EXPLORING

- Gfarm storage can be also explored via file search dialog.
  - Need to setup on preferences of Job Builder
  - Require gfarm-DSI on the gfarm server side





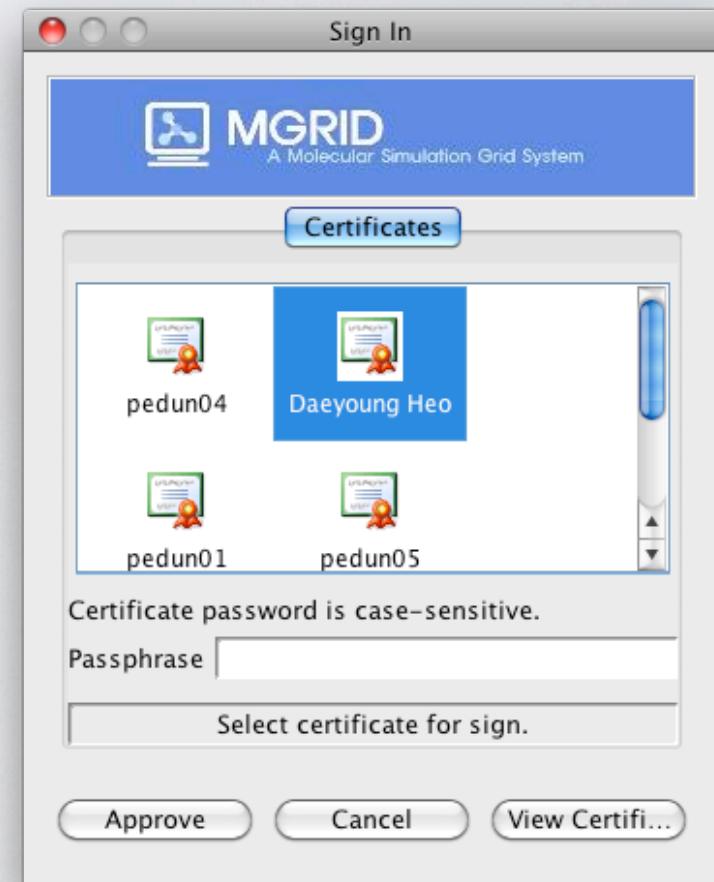
# MGrid Tutorial B

Customize Job Builder  
for my grid environments

# CONVINENT WAY OF SIGN IN

## - SAFEBOX -

- GUI tool for sign-in.
- Easy management of certificates.
- Support sign-in on mobile device: delegate a certificate to ID and password system.
- Sharing user preferences between MGrid applications.



# SAFEBOX

- More safe
  - In safebox, credential is only stored in memory, while grid-proxy-init is stored to filesystem.
- More convenient for managing multiple certificate.





# MGrid Tutorial A

Portal Configuration

TO ACCESS SIMULATION  
DATA AS IF REGULAR FILE ON  
LOCAL STORAGE

MGrid Portal

http://service.mgrid.or.kr:80/service/gridsphere?cid=mgridws

Mgrid Portal pragma19 - Google 검색

MGRID A Molecular Simulation Grid System

Welcome | Certificate Manager | Workspace | Job Monitor | Blogging | RIMES | Document | Tutorial | About

Logout Welcome, Daeyoung Heo

Workspace Credential Manager

New Project

My Projects

- All
- /s/
- koex1
- koex2
- RIMESTest
- TEST

Labels

- BASH
- DEVELOP
- EXAMPLE
- free\_ec2
- NAMD
- NAMDWAPPER
- PARAGMA18
- RIMES
- RIMESWrapper
- with

Navigation

Trials

Displaying trial 1 - 3 of 3

IDX Status Date

- 0 Y Tue 4:11 pm  
\*\*empty description\*\*
- 1 Y 2010-02-26 Fri ...  
Execution Tool Test
- 2 Y Tue 3:49 am  
RIMES Test (DDC file) #1

Run Delete Download Blogging Option Filter: Search a Trial Go

NAMD(ubq\_ws\_eq) with RIMES

OU=OOU=AGC/OU=KMU/OU=cs.kookmin.ac.kr/CN=Daeyoung Heo MGrid Job Builder v2.0

PARAMETERS

| INPUT FILES                            | OUTPUT FILES   | TEXT PARAMETERS        |
|--|--|------------------------|
| par_all27_j<br>ubq_ws.pd<br>ubq_ws.psi | ubq_ws_ec<br>ubq_ws_ec<br>ubq_ws_ec<br>ubq_ws_ec<br>ubq_ws_ec<br>ubq_ws_ec | minimize<br>temperatur |

SCRIPT

```
#####
## JOB DESCRIPTION
#####

# Minimization and Equilibration of
# Ubiquitin in a Water Sphere

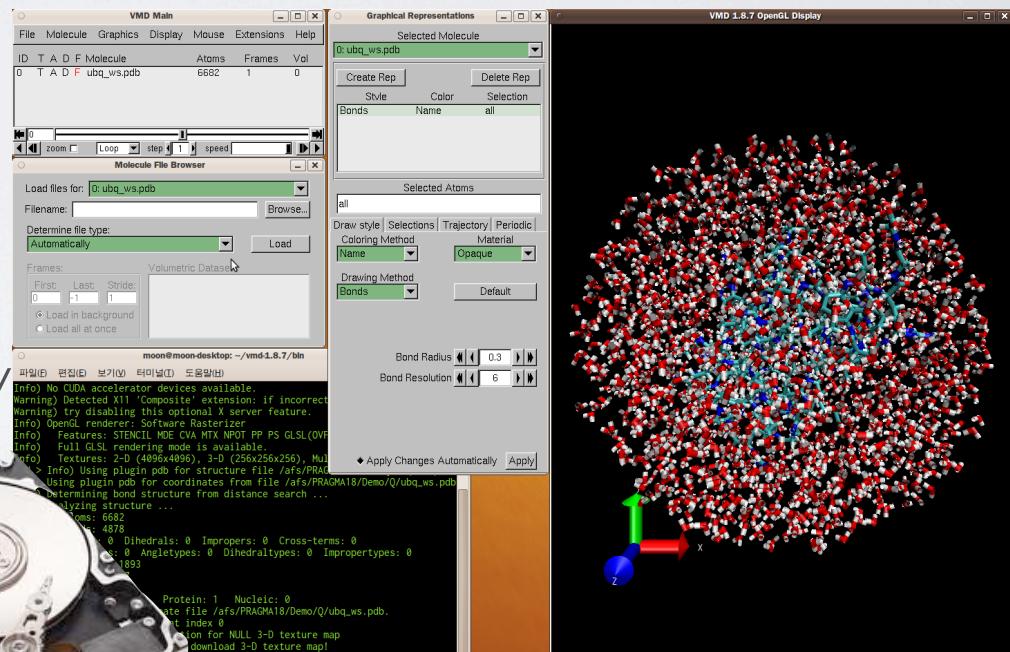
#####
## ADJUSTABLE PARAMETERS
#####
```

September 15, 2010

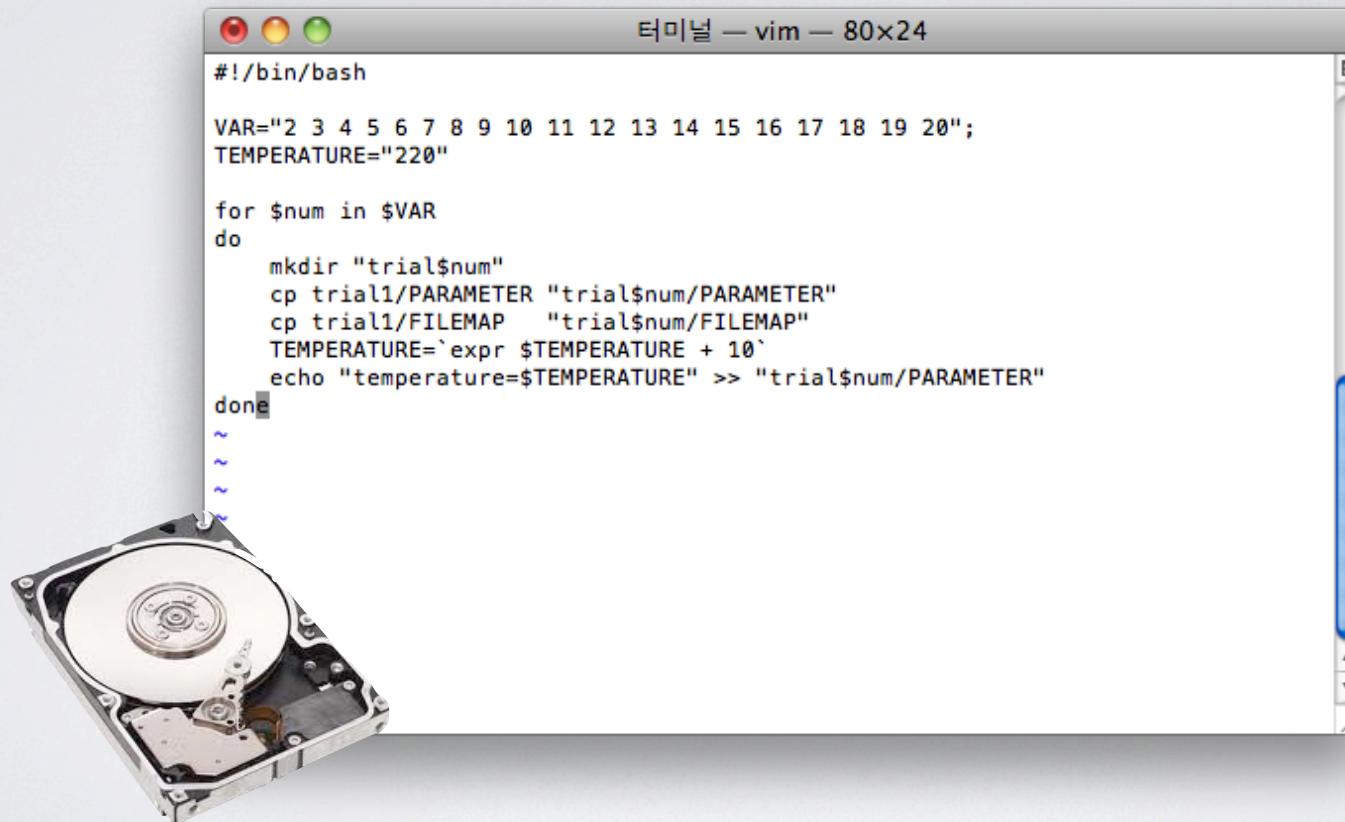


# FOR EXAMPLE: VMD

- Access to simulation data without download from portal nor modifying legacy application.



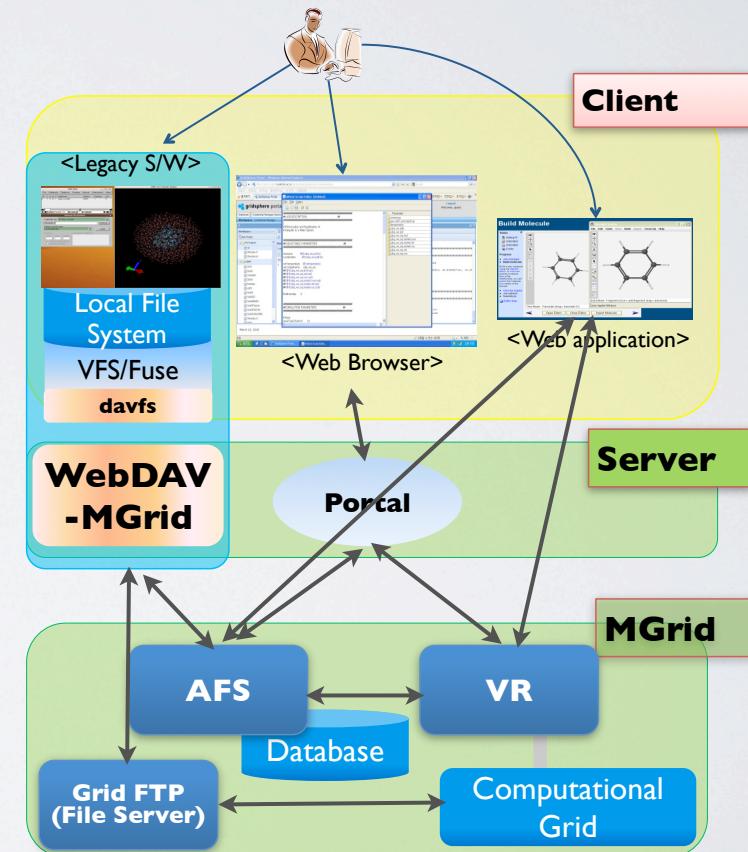
# PROGRAMMABLE PARAMETER SWEEPING FOR BULK



# SIMPLE REPORTVIEW

# BY USING WEBDAV

- Convert to service object to file or directory.



# INTEGRAGTE SNS FOR SHARING: SUPPORT BLOG.

- Publish to your blog
  - Using Template Page
  - Added file links.

The screenshot shows a blog post titled "daeyoung heo". The post header includes "Home", "RSS Feed", and "Comments Feed". The date is listed as "2010년 9월 13일 월요일 10 comments". Below the header, there are three tables:

- Simulation Information -**

|                    |  |
|--------------------|--|
| Job Title          | activefolder   |
| Glyco-Trivial Name |  |
| Classification     | Biological Glycan  |
| Authors            | / O=Grid/ OU=AGC/ OU=KMU/ OU=cs.kookmin.ac.kr/ CN=Dae young Heo          |
| Citation           |  |
| History            |  |
| Computation Method | MD   |
| Canonical Format   |  |
| Active Project     | Conformational database of glycan molecules<br>Avian flu-related glycans |
- Simulation Parameter -**

|                     |                           |                            |                           |
|---------------------|---------------------------|----------------------------|---------------------------|
| Force Field         | Simulation Program        | Solvation                  | PBC                       |
| CHARMM-CSFF         | CHARMM                    | Water                      | YES                       |
| Crystal Type        | Ensemble                  | Dielectric Condition       | Long-Range Electrostatics |
| Cubic               | NPT                       | Constant Dielectric        | Ewald Summation           |
| Temperature Control | Pressure Control          | Nonbonding Cutoff Distance | Dielectric Constant       |
| Hoover              | Langevin piston           | 15                         | 1                         |
| Time Step (fs)      | Total Simulation Time(ns) |                            |                           |
| 2                   | 30                        |                            |                           |
- Simulation File Parameter -**

|  |  |
|--|--|
|  | free_eq.restart.xsc<br>A.prmtop<br>free_eq2.xst<br>free_eq.restart.coor<br>A.innrd |
|--|--|

MORE...

# PLSI

- Partnership & Leadership for the nationwide Supercomputing Infrastructure



# DEPLOYING ON PLSI

- Under the working.

The screenshot shows the login interface for the MGrid system. At the top, there's a logo for 'PLSI' (국가 슈퍼컴퓨팅 공동 활용 체제 구축) and a language selection 'English'. Below that is a 'Home' link. The main title is 'MGrid: A Molecular Grid System' followed by a subtitle 'An Application Grid System for Robust, High Throughput Molecular Simulation.' To the right is a login form with fields for 'User Name' and 'Password', a 'Remember my login' checkbox, and a 'Login' button. There's also a link 'Forgot your password?'. At the bottom of the page, there are logos for KU (Konkuk University), KISTI (Korea Institute of Science and Technology Information), and KMU (Kyung Hee University). The footer contains the text 'PLSI 국가 슈퍼컴퓨팅 공동 활용 체제 구축' and 'KISTI 국립 과학 기관 협력 활용 체제 구축'.

|   | Institute                        | CPU         | Node       | Tflops      |
|---|----------------------------------|-------------|------------|-------------|
| 1 | <b>KISTI</b>                     | <b>2352</b> | <b>152</b> | <b>38.3</b> |
| 2 | <b>KIST</b>                      | <b>152</b>  |            | <b>1.82</b> |
| 3 | <b>Seoul National University</b> | <b>112</b>  | <b>2</b>   | <b>0.98</b> |
| 4 | <b>Pusan National</b>            | <b>112</b>  | <b>16</b>  | <b>0.67</b> |
| 5 | <b>TongMyong University</b>      | <b>152</b>  | <b>3</b>   | <b>1.71</b> |
| 6 | <b>Pukyong National</b>          | <b>256</b>  | <b>2</b>   | <b>1.43</b> |
| 7 | <b>GIST</b>                      | <b>256</b>  | <b>2</b>   | <b>1.43</b> |
| 8 | <b>UNIST</b>                     | <b>648</b>  | <b>40</b>  | <b>6.13</b> |
| 9 | <b>Konkuk University</b>         | <b>?</b>    | <b>?</b>   | <b>?</b>    |
|   |                                  | <b>4040</b> |            | <b>50.5</b> |

# SOFTWARES

- Amber
- NAMD
- Charmm ( for internal user)
- VASP
- Gaussian 03 ( for internal user)
- Bash, python, etc...

**PLSI** 국가슈퍼컴퓨팅공동활용체제구축

# PLSI-MGRID



건국대



기상청



동명대



부경대



부산대



부산테크노파크



서울대



KISTI  
한국과학기술연구원



KISTI  
한국과학기술정보연구원



GIST



UNIST