A Catch-All Science Gateway Portal for Malaysia Research Communities

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Introduction

- In Malaysia, the National Grid Initiative/Infrastructure is called Academic Grid Malaysia.

- The Academic Grid Malaysia is an open access distributed computing infrastructure Open to any Malaysian Academia from institutions and organizations that are recognized by respective ministries to be involved/ associated in/with Distributed-, Grid-, Cloud- and Emerging Computing Applications/Projects

- The Academic Grid Malaysia provides opportunities to the user communities to run their existing applications more quickly and efficiently, and also to create ambitious new applications, without investing in extra hardware, and software resources.

Problems

- However, converting existing applications into Grid applications, and also creating new applications, currently requires significant Grid knowledge, which many users do not have.

- Most of the user communities that have used Grid are accessing the resources via Linux command line. However some of the users are not familiar with Linux command line, moreover it becomes "extra" work for them after their actual research work.

- This is one of the reasons of low Distributed Computing Infrastructure (DCI) adoption among research communities in Malaysia.

Solution

- In order to solve the problems, we developed a catch-all science gateway portal as the "medium" to access the Academic Grid Malaysia infrastructure.

- Catch-all here means the portal is not specifically developed/ designed for a specific science application. The portal is generic and is able to host many science applications.

- By providing science gateway portal, it is hoped that user communities no longer face problems and there is a common set standard in accessing the DCI (i.e. NGI Malaysia).

User community and scientific area targeted by the Science Gateway

- There are three major user communities that are targeted by the science gateway:

  - Life science is still one of the main research focus in Malaysia, hence many researchers are doing research on that particular field (i.e. Computational Biology and Chemistry). However, most of them are still using their own personal workstation to do simulation that could take days to complete. Some of the reason why they have yet to adopt the DCI approach is because it requires resources which at this point of time they do not have.

  - Creative industry (i.e. Multimedia) is one of the area that is actively supported by the government of Malaysia. Hence many academic institution offers programs in this field of study. However, some activities require decent hardware for rendering and not all academic institution can afford this requirement.

  - Engineering domain generally has adequate resources in running their simulation/application in High Performance Computing. However, most of the users rely on commercial/licensed Engineering software which is costly and has some limitation in the number of users and hardware (i.e. servers).
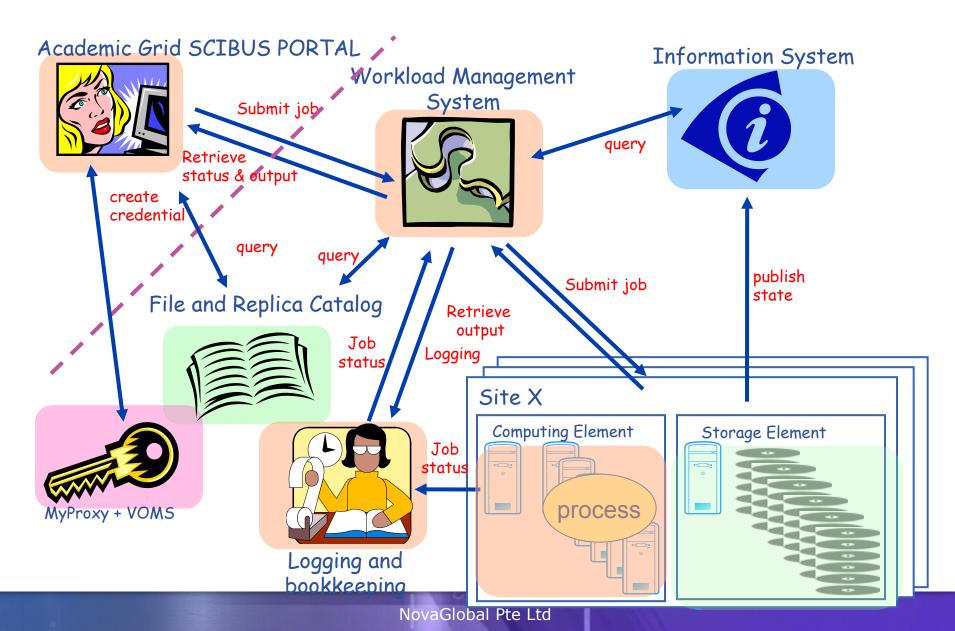
Methodology

- Long before the science gateway for Academic Grid Malaysia is available, NVG Scientific have developed a portal consisting of Bioinformatics application portlets that is currently hosted at the National University of Singapore.

- However the portal is not suitable to be implemented at the Academic Grid Malaysia infrastructure because most of the portlets was hardcoded to work with the LSF software.

- Instead, we took the design of each portlet and re-write it according to WS-PGRADE/gUSE+ASM framework.

Methodology

- The segregation of the presentation and workflow layer in WS-PGRADE/gUSE framework gives us some benefit:

    1. The web programmer can focus on developing/coding the portlet
    2. The workflow designer can focus on developing/creating the application workflow that is the actual "workhorse" of the portlet.

- The workflow shall be tested and validated by the workflow designers and the end-users (volunteer) from each user communities before the web programmer "glues" the presentation layer and the workflow together.

- After the web programmer glued the presentation layer and the workflow together, the portlet goes to the second validation test before it is released to the public
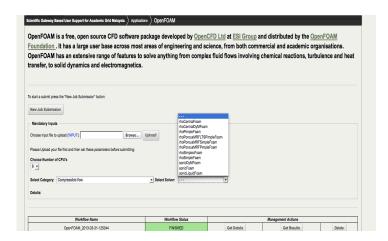
How does it works?

Screenshot

Fact Sheet

- Portal homepage : http://scibus.cict.utm.my

- Portal Framework : WS-PGRADE/gUSE version 3.5.5

- Programming API : ASM 3.4

- Operating System : Scientific Linux 6.2

- Grid Middleware : EMI Middleware UI version 2.0

- Applications: Autodock4, AMBER, NWChem, GROMACS, FastDNAml, Phase, Clustalw-MPI, BLAST* , Muscle , OpenFOAM ,Blender*, Multidendrograms, PROSPECT, NAMD*, Glimmer*

* Will be released soon.

Summary

- The NGI Malaysia provide opportunities to the user communities to run their existing applications more quickly and efficiently, and also to create ambitious new applications, without investing in extra hardware, and software resources.

- Most of the user communities that have used Grid are accessing the resources via Linux command line.

- However this becomes a problem since not all of the users has Linux skills. This is one of the reasons for low Distributed Computing Infrastructure (DCI) adoption among research communities in Malaysia.

- By providing them a science gateway, it is hoped that user communities no longer face any problem in accessing the DCI (i.e. Academic Grid Malaysia) and also increase the adoption of the DCI technology among research communities in Malaysia

Acknowledgement

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    - Centre for Information and Communication Technology – Universiti Teknologi Malaysia for providing us resource to access to the Malaysia Research and Education Network.

Demo

- Login to : http://scibus.cict.utm.my
- Username: demo@novaglobal.com.sg
- Password: 45scibus123