



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).

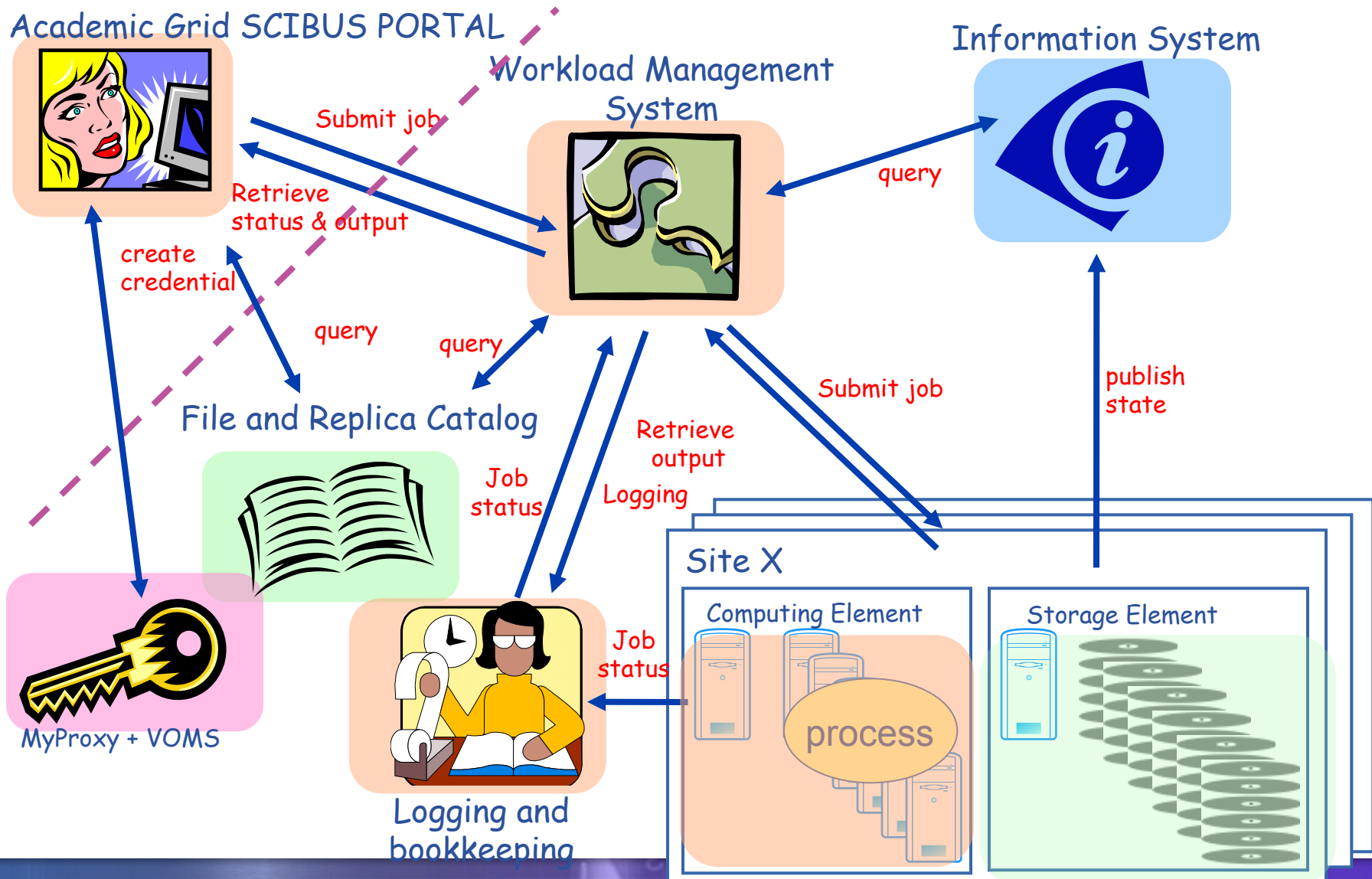
Methodology

- 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

The screenshot shows the homepage of the Scientific Gateway Based User Support Portal for Academic Grid Malaysia. The header includes logos for NOVA GLOBAL, ACADEMIC GRID MALAYSIA, UTM, and SCI-BUS. A navigation bar contains links: Welcome, Applications, Storage, Settings, Publications, Help, and Security. Below the navigation bar, a breadcrumb trail reads: Scientific Gateway Based User Support for Academic Grid Malaysia > Welcome. The main content area features a heading "Welcome to the Scientific Gateway Based User Support Portal for Academic Grid Malaysia" followed by two paragraphs of text describing the SCI-BUS project and its goals. At the bottom right, it says "Powered By Liferay".

NOVA GLOBAL ACADEMIC GRID MALAYSIA UTM Centre for Information and Communication Technology SCI-BUS

Welcome Applications Storage Settings Publications Help Security

Scientific Gateway Based User Support for Academic Grid Malaysia > Welcome

Welcome to the Scientific Gateway Based User Support Portal for Academic Grid Malaysia

The SCI-BUS project aims to ease the life of e-Scientists by creating a new science gateway customization methodology based on the generic-purpose gUSE/WS-PGRADE portal family. The customized science gateways will enable scientists to focus on their work and exploit resources of main Distributed Computing Infrastructures (DCIs) without the need to deal with the underlying infrastructures' details. SCI-BUS is supported by the EU FP7 Capacities Programme under contract n°RI-283481.

NovaGlobal (through its subsidiary: NVG Scientific Sdn Bhd) has been selected as one of subcontractor for the SCI-BUS project. This selection will open new opportunity for cross border academic-industry collaboration between Malaysia and Singapore as well as with other ASEAN and European countries.

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Powered By Liferay

This screenshot shows the "Applications" menu open in the portal. The menu lists several applications: AMBER, Autodock, ClustalW, FastaDNAMl, GROMACS, MUSCLE, NWChem, OpenFOAM, PHASE, and Multidendrograms. The background shows the same header and navigation bar as the first screenshot, with the "Welcome" page content partially visible behind the menu.

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This screenshot shows the "OpenFOAM" application interface. It includes a description of OpenFOAM as a free, open source CFD software package. Below the description, there is a "New Job Submission" button and a "Mandatory Inputs" section. The "Mandatory Inputs" section contains a "Choose input file to upload (INPUT)" field with a "Browse..." button and an "Upload" button. Below this is a "Please Upload your file first and then set these parameters before submitting:" section. It includes a "Choose Number of CPUs" field with a dropdown menu set to "8". There is also a "Select Category" dropdown menu set to "Compressible flow" and a "Select Solver" dropdown menu. At the bottom, there is a table showing workflow details.

Scientific Gateway Based User Support for Academic Grid Malaysia Applications OpenFOAM

OpenFOAM is a free, open source CFD software package developed by OpenCFD Ltd at ESI Group and distributed by the OpenFOAM Foundation. It has a large user base across most areas of engineering and science, from both commercial and academic organisations. OpenFOAM has an extensive range of features to solve anything from complex fluid flows involving chemical reactions, turbulence and heat transfer, to solid dynamics and electromagnetics.

To start a submit press the "New Job Submission" button:

New Job Submission

Mandatory Inputs

Choose input file to upload (INPUT) Browse... Upload

Please Upload your file first and then set these parameters before submitting:

Choose Number of CPUs 8

Select Category: Compressible flow Select Solver:

Workflow Name	Workflow Status	Management Actions
OpenFOAM_2013-03-31-12544	FINISHED	Get Details Get Results Delete

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

- Herewith we would like to thank you:
 - SCI-BUS project for providing us research grant to develop the Science Gateway for Research Communities in Malaysia. SCI-BUS is supported by the EU FP7 Capacities Programme under contract n°RI-283481. NVG Scientific Sdn Bhd has been appointed as one of SCI-BUS subcontractor.
 - 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