The Griffith University Computational Resources Framework

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**THE FRAMEWORK CONCEPT**

The Griffith University Computational Resources Framework will allow researchers to use High Performance Computing (HPC) resources to process, model, simulate, project and predict in a more user friendly manner by masking the underlying complexity involved. This will be achieved through the development of simple, secure and user friendly Graphical User Interfaces (GUI) that will allow submission of various job types to be processed by various computing resources. This Project has primarily been developed by students undertaking the Work Integrated Learning (WIL) Industrial Affiliates Project course at Griffith University.

**THE AUTOMATED COMPUTATIONAL ANALYSIS OF BIOMOLECULAR DATA (ACABD) PROJECT**

This project designed, implemented and tested a user friendly submission portal for Not Another Molecular Dynamics (NAMD) jobs onto Griffith University HPC resources. This project used the web-based GUI content management system, Drupal. A Globus framework was also incorporated to certify the system was being used appropriately and to direct the flow of data within the system. Scripts were also created to facilitate communication between the GUI user layer, the Globus middleware layer and the services layer (comprised of a metadata database, NAMD enabled processor, data repository and authentication services). Upon job submission the user can navigate through the GUI to view the jobs they have submitted. From the GUI they can also view the specific details of each job, such as job status.

**THE E RESEARCH COMPUTATIONAL FRAMEWORK PROJECT**

This Project extends the ACABD Project to include a dedicated iRODS data repository and automated email notification at job completion. iRODS was successfully integrated into the existing middleware layer and interoperable authentication procedures were implemented between iRODS password authentication and ACABD certificate authentication by mapping the username and password from ACABD to iRODS. This provides a Single Sign-on service. The researcher’s input and output files can be accessed through an iRODS GUI within the ACABD website. This project also canvassed a variety of visualisation options for future integration into the framework. This would allow interpretation of results within the portal environment and thus minimise the necessity for large data transfer and local file storage.