



APCF Computational Cluster a large computing resource in running proteomic searches

Introduction

The Australian Proteomics Computational Facility (APCF) provides an automated computational facility for all proteomics researchers in Australia as well as access from abroad. This enables researchers to access world-class proteomics computational resources and databases. Funding is provided by the Australian National Health and Medical Research council (NH&MRC).

The APCF is managed by a collective of Australian academic researchers from all states and territories with interests in proteomics, and is advised by local and overseas experts in the field. The APCF is a unique consortia to supply mass spectrometry centric data analysis, delivered on a national scale.

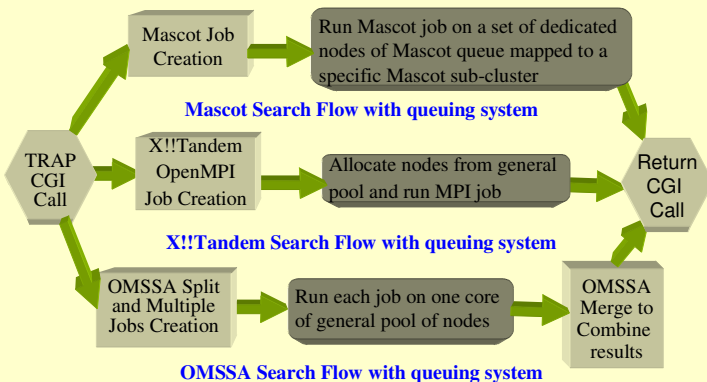
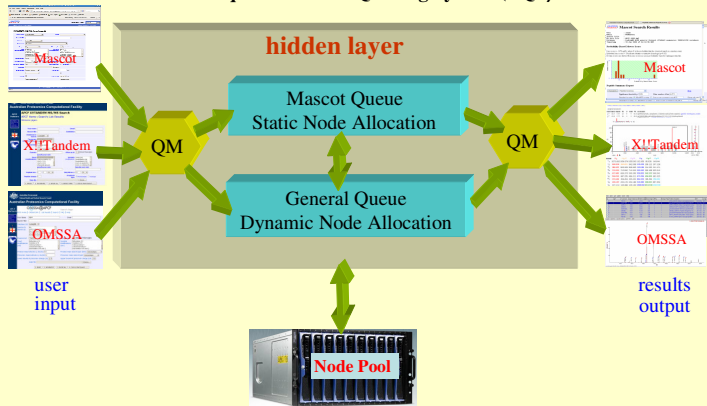
APCF computational cluster is the backbone for supporting computational needs of the Australian Proteomics Community by maintaining international standards in the field of High-Performance Computing. The facility has enormous computational power with 128 dedicated computational nodes with 1024 cores with over a half-dozen systems to manage all aspects and act as gateway systems to the computational nodes.

APCF Cluster Queuing System

- The APCF has constructed a sophisticated queuing system, which allows running multiple MS/MS databases searches concurrently, without competition, for best utilization of computational resources combined with fault-tolerance to ensure the integrity of each submitted search.
- The queuing system has a mapping capability which provides seamless computational power to the needs of the APCF search algorithms of Mascot, X!!Tandem and OMSSA.
- The APCF queuing system has a scalable scheduler which allows for system scheduling of jobs according to the requirements and priorities of the computational needs.
- APCF add-ons allow to resubmit failed searches by reallocating computational nodes dynamically without users knowledge to the queuing system which makes the system fault-proof.

Unified Access to APCF computational cluster

APCF Torque/PBS/Maui Queuing System (TQS)



Queue Manager (QM) and Queue Scheduler (MAUI)

Queue Manager for Torque/PBS (QM) provides queuing services to the system. The Maui Scheduler is a policy engine which allows control over when, where, and how resources such as processors, memory, and disk are allocated to jobs and also help to intelligently optimize the use of these resources.

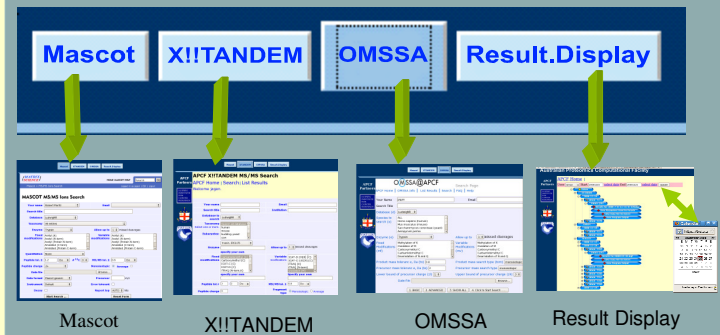
Advantages of using Intelligent queues

- Highly scalable
- High Fault tolerance
- No limit on number of job submissions
- High availability of system
- Concurrent runs with multiple resources benefit users to return search results quickly
- Allows to distribute workload over to low usage timings
- Allow to run more priority jobs in ahead of low priority jobs
- Dynamic allocations of resources makes the system more robust
- User doesn't need to learn any new technology to use APCF facilities

APCF Interfaces (UNITE & UNIWI) with 128bit Security

- Specially designed web based software that resides on the gateway systems hidden from the user, provides a unified interface to receive jobs (searches) from range of tools including the APCF designed automated interface "UNITE", Mascot Daemon and standard web pages in a highly secure manner through high 128 bit SSL encryption and translate them into jobs for queuing system in a seamless manner.
- APCF UNITE provides a Unified interface to Mascot, X!!Tandem and OMSSA searches. Multiple files can be searched with multiple algorithms, all with a single click.
- APCF UNified Web Interface (UNIWI) provides Unified web access to all the search algorithms and search results from the same web page instance.
- Create customized result views and their listings for individuals or entire group from a Unified Web Interface page with a popup window to select dates in a user friendly manner.
- A group security system allows users to share results.
- Security certificates are signed and validated by an International authority in securing web sites.
- The security mechanism installed at the APCF cluster not only validates user's credentials but also provides secure communication channels between the users system and the APCF.

APCF UNified Web Interface (UNIWI)



APCF Highlights and Future Extensions

- The APCF constructed system integration and scheduling is a world's- first proteomics data analysis facility that allows researchers to seamlessly access multiple industry-standard MS/MS databases searching algorithms remotely, simultaneously and securely at the facilities of the APCF.
- Easy access to all data, including search parameters, spectrum files and output files.
- By default every user can have access to standard sequence databases LudwigNR, IPI and SwissProt but also possible to add group specific databases for any group on request.
- The facility has been designed to scale well for the future needs not only in the storage space but also in computational power with enterprise level tools developed around the world following the International standards.
- Users can access the APCF using UNITE or UNIWI from anywhere in the world using standard Web Browsers like Internet Explorer, Firefox and Safari from any type of operating systems Windows, Linux, UNIX and Mac etc., with a standard Internet Connection.