

Computational and Data GRIDS

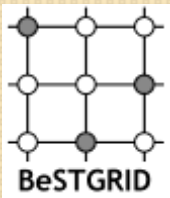
Bringing the HPC Resources to NZ Researchers

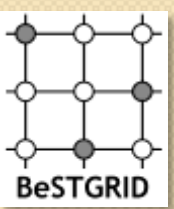
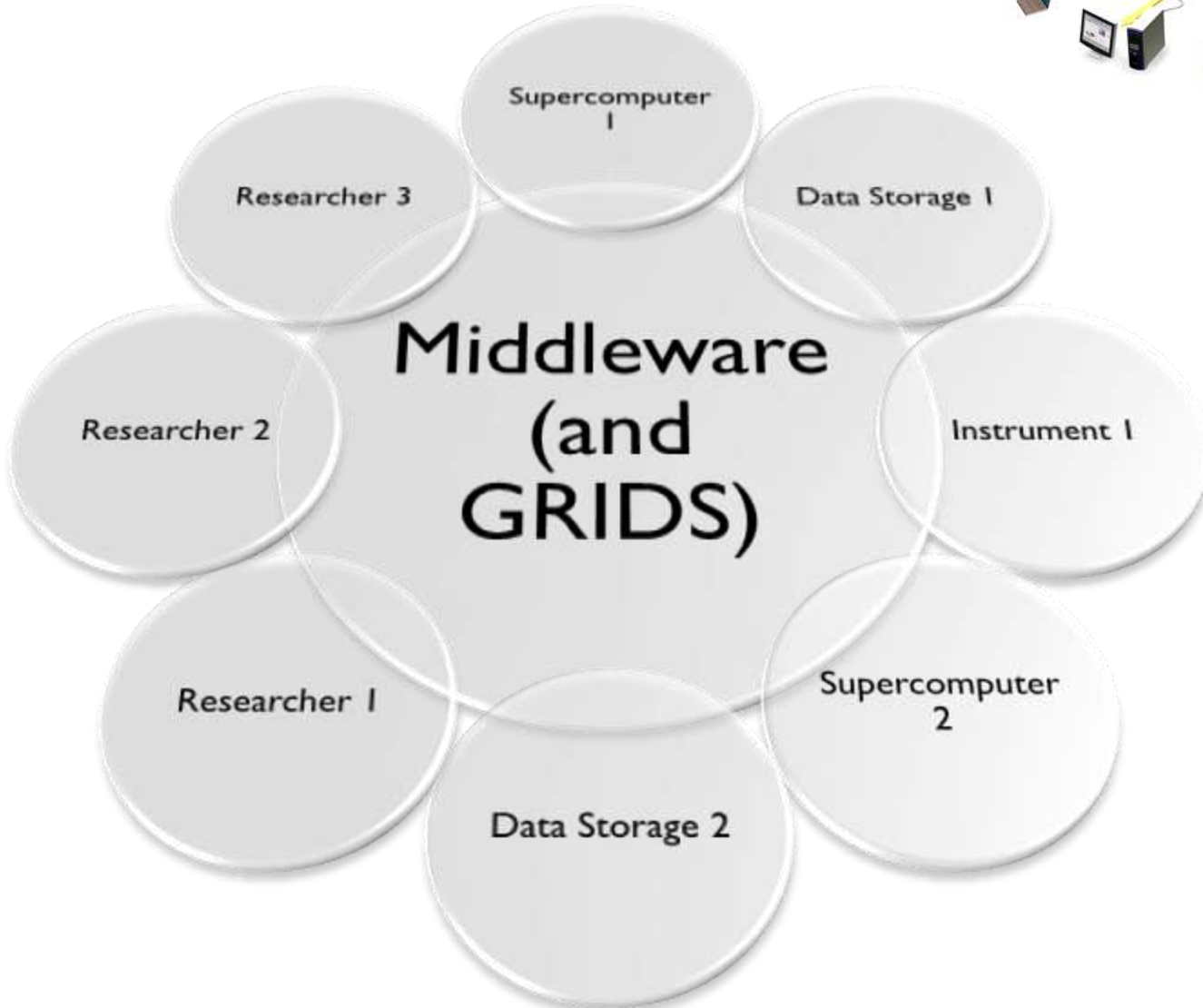
BeSTGRID Goal: to streamline access

Connect the resources and transparently present them to the community

To match users and their jobs to the best computational resources for their needs

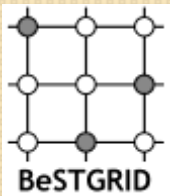
“Not-so-low-hanging fruit”

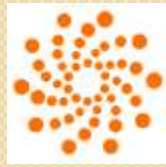




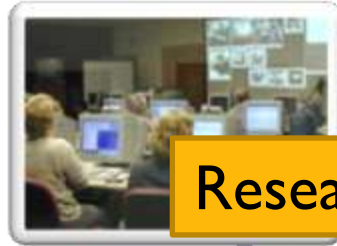
Strategy: Alignment with APAC GRID

- APAC Grid – Australian Partnership for Advanced Computing GRID
- BeSTGRID will aim to **align** technically with APAC GRID
- Will facilitate future **interoperability** and possible partnership in future

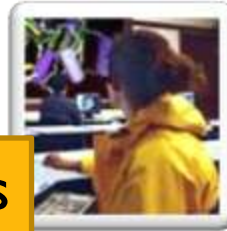




APAC National Grid

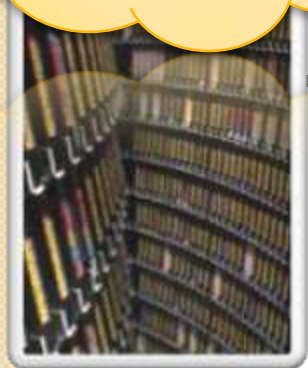


Research Teams



Sensor Networks

Data Centres



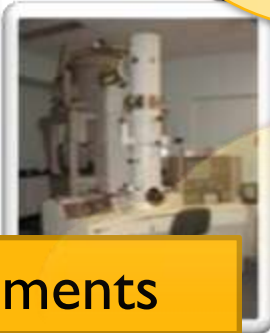
National Grid
a virtual system of computing, data storage and visualisation facilities



Other Grids:
Institutional
International

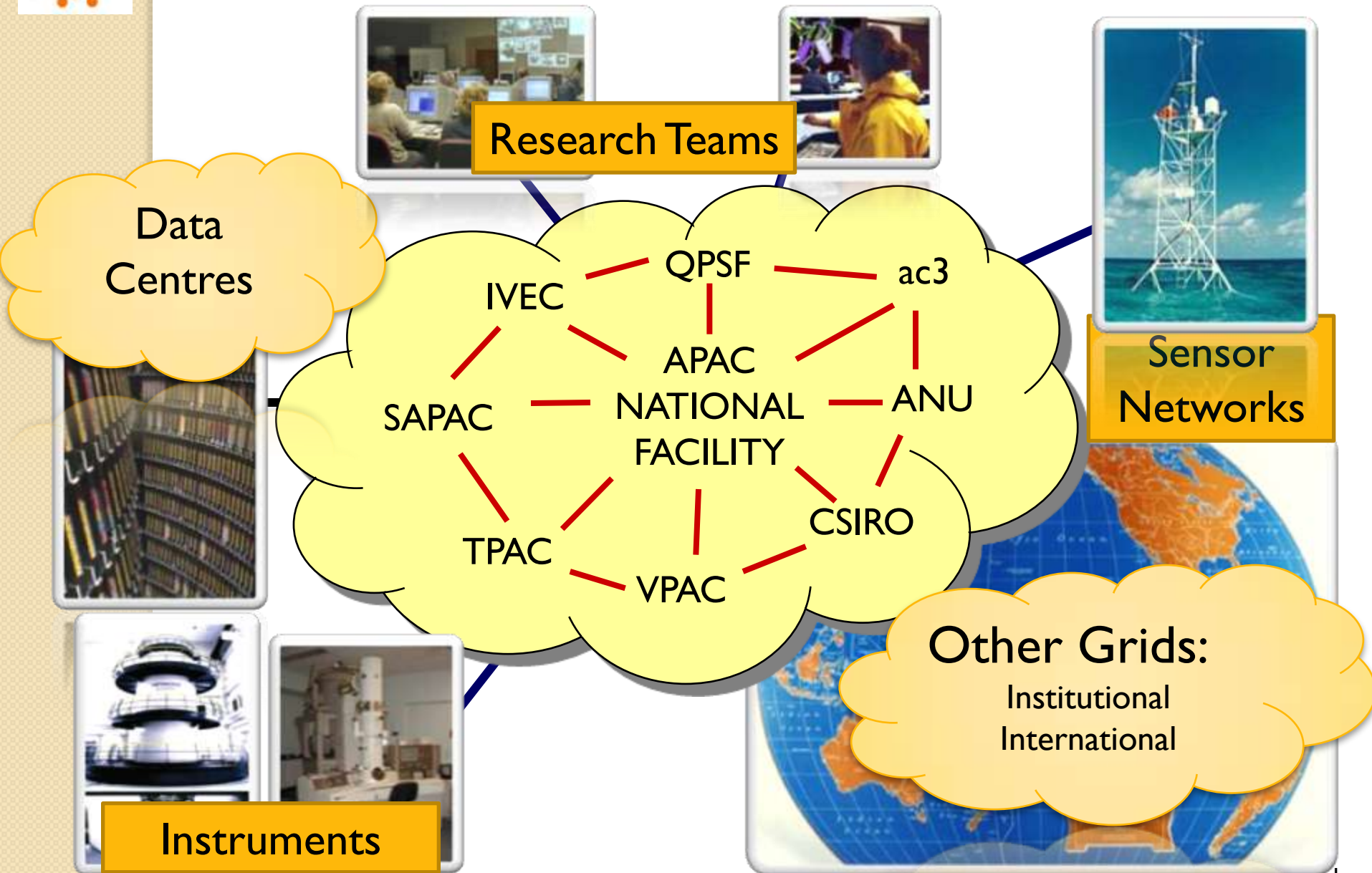


Instruments





APAC National Grid



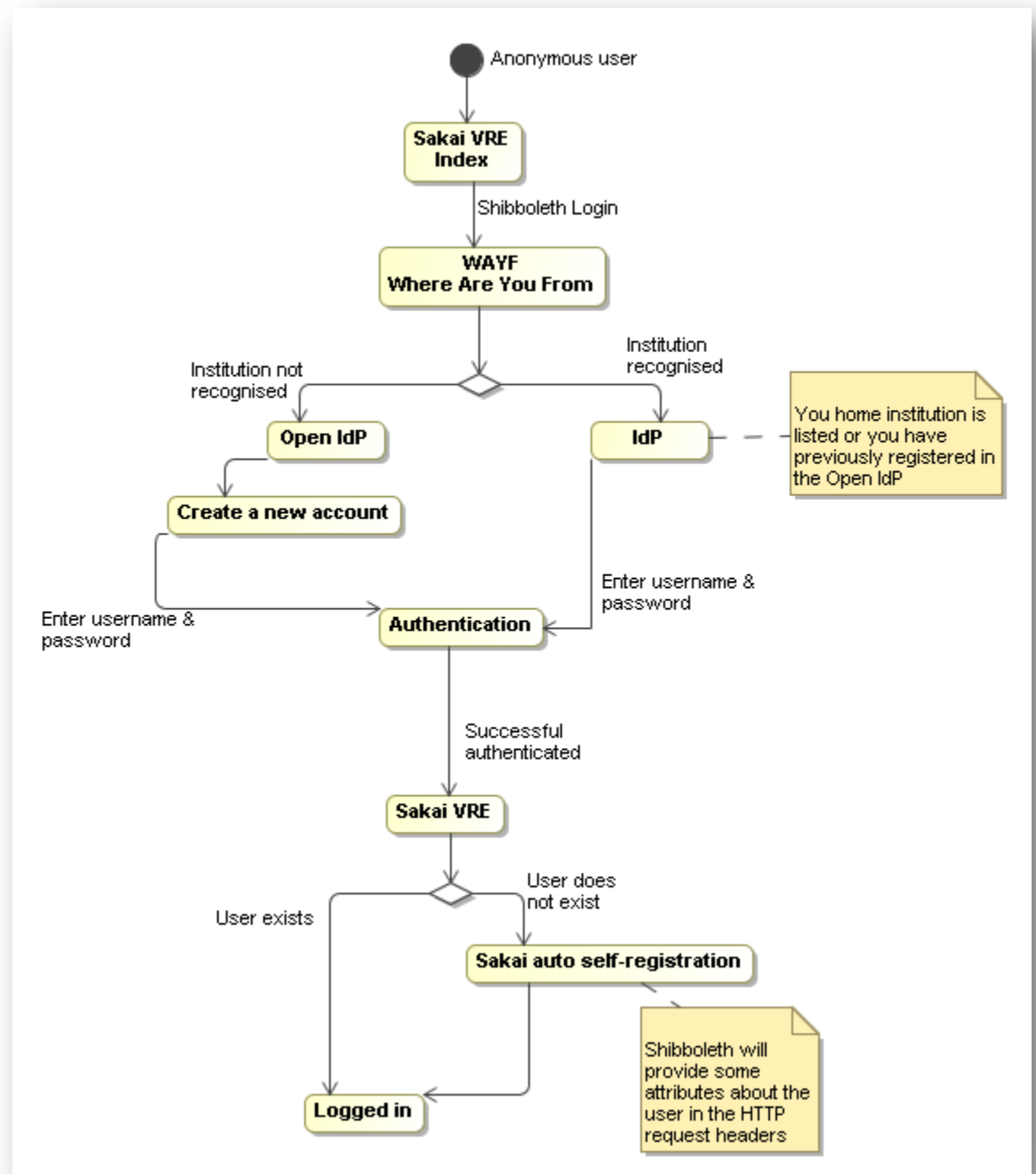
Federated Identity and Access Management



- Australian Access Federation (related to MAMS)
- Shibboleth
- APAC Certificate Authority

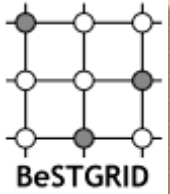


Shibbolised Sakai-VRE

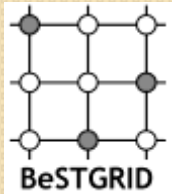


You home institution is listed or you have previously registered in the Open IdP

Shibboleth will provide some attributes about the user in the HTTP request headers



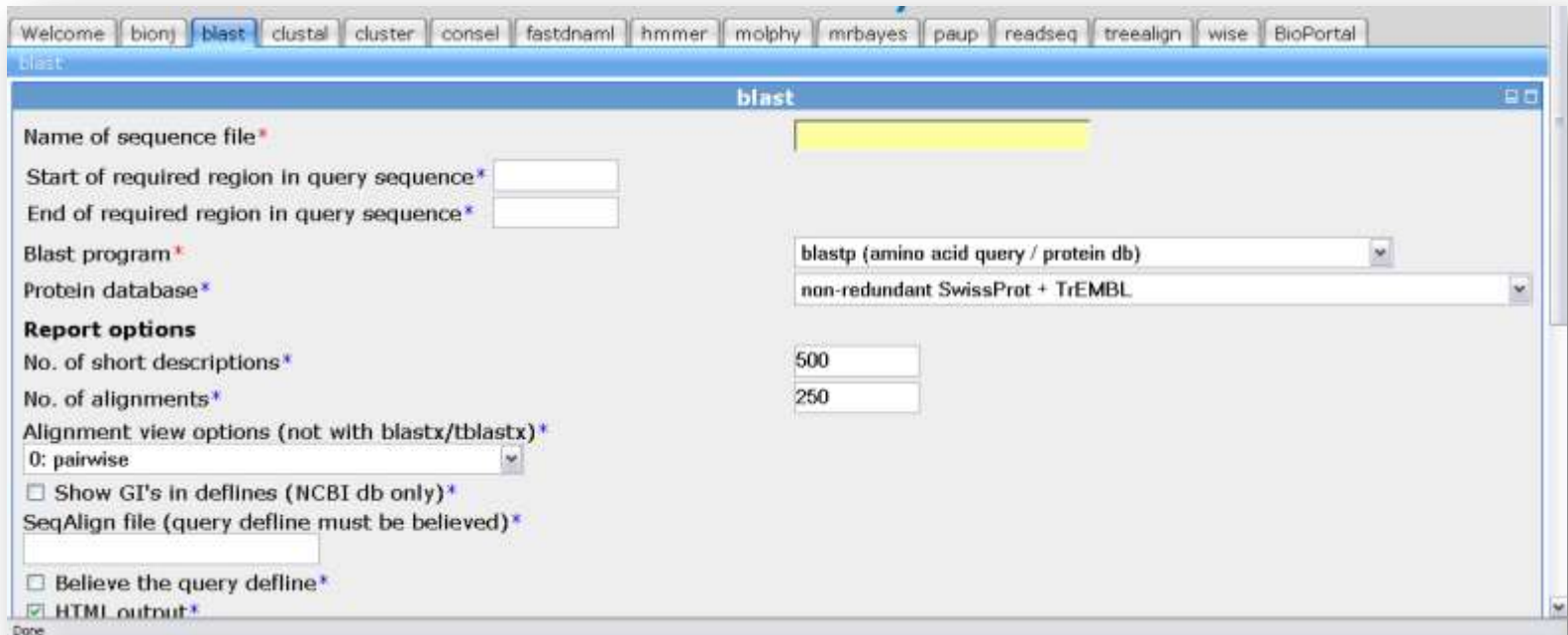
Portals and Web Services for the GRID



BeSTGRID's NZ Bioportal

The screenshot shows a web browser window with a navigation bar at the top containing links: Welcome, bionj, blast, clustal, cluster, consel, fastdnaml, hmmer, molphy, mrbayes, paup, readseq, treealign, wise, and BioPortal. The main content area is titled "Paup Portlet" and features a large heading "Paup". Below the heading is a navigation bar with tabs: Job Submission (selected), Block Form Creation, Files and Results, Instructions, and Preferences. The "Job Submission" section contains a "Paup Command File" field with a "Browse..." button, and "HPC Resources" with input fields for "Num. CPUs: 1" and "CPU Hours: 9999". The "Instructions" section contains text: "Please select the Paup Command File you wish to run and adjust the CPU parameters before submitting. Please note that the Paup Command file that you select must contain only 1 Paup Command section." and "For more detailed instructions please select the Instructions Tab from the Navigation Bar, or the question mark in the Title Bar of this window." At the bottom of the form are buttons for "Reset to default values" and "Submit File to Paup".

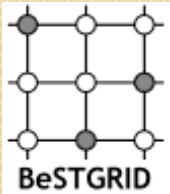
BeSTGRID's NZ Bioportal



The screenshot shows a web browser window with a navigation bar at the top containing tabs for 'Welcome', 'bionj', 'blast', 'clustal', 'cluster', 'consel', 'fastdnaml', 'hmmer', 'molphy', 'mrbayes', 'paup', 'readseq', 'treealign', 'wise', and 'BioPortal'. The 'blast' tab is active. The main content area is titled 'blast' and contains the following fields and options:

- Name of sequence file*: [Yellow highlighted text box]
- Start of required region in query sequence*: [Input field]
- End of required region in query sequence*: [Input field]
- Blast program*: blastp (amino acid query / protein db) [Dropdown menu]
- Protein database*: non-redundant SwissProt + TrEMBL [Dropdown menu]
- Report options**
- No. of short descriptions*: 500 [Input field]
- No. of alignments*: 250 [Input field]
- Alignment view options (not with blastx/tblastx)*: 0: pairwise [Dropdown menu]
- Show GI's in deflines (NCBI db only)*
- SeqAlign file (query defline must be believed)*: [Input field]
- Believe the query defline*
- HTML output*

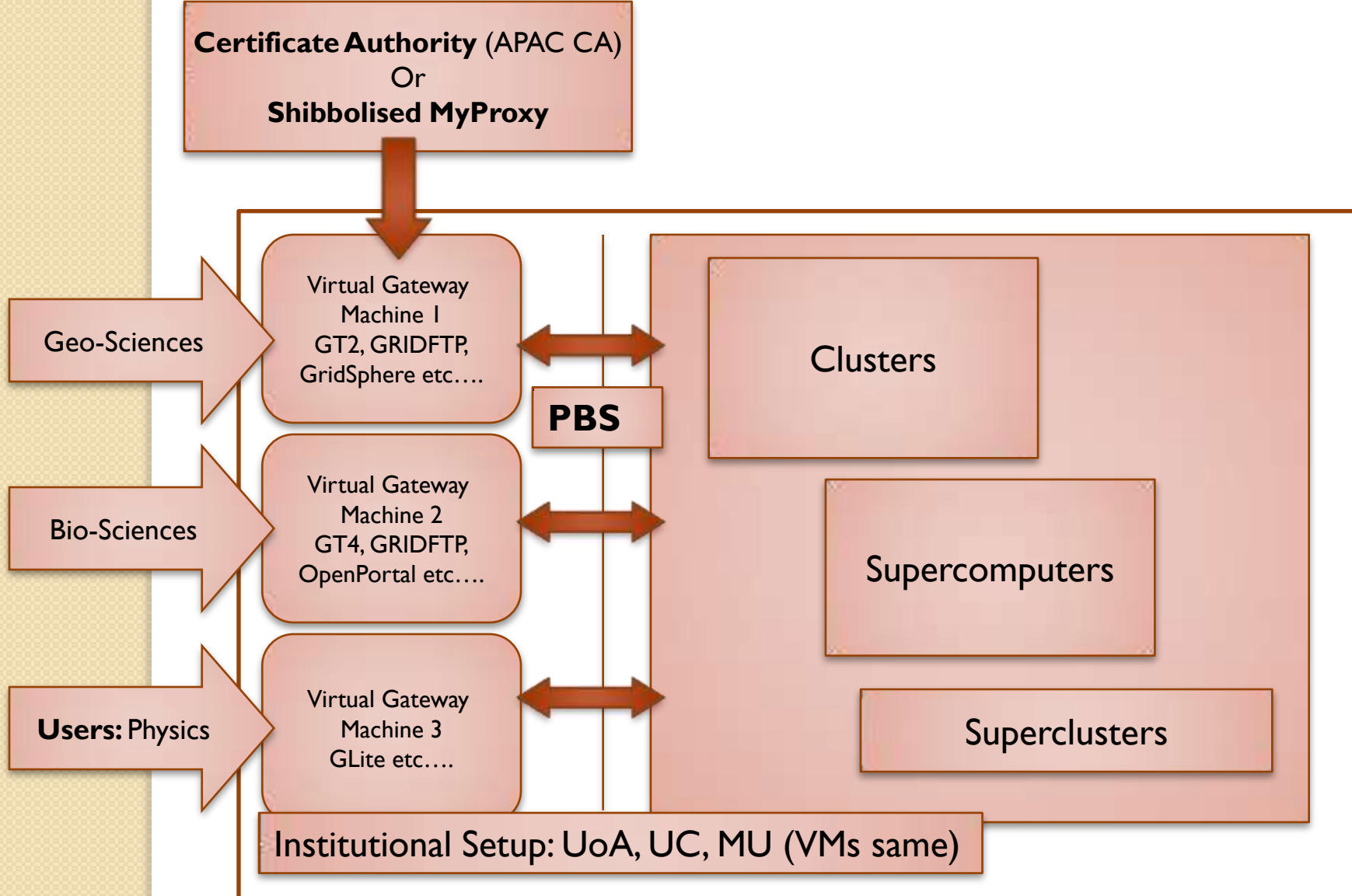
Done



Virtual Gateways of APAC Grid

- Key APAC Grid Feature: Use of “Virtual Gateways” for each discipline (involving Xen Virtual Machines)
- Virtual Gateways provide compatibility with both US and European GRID efforts (i.e. Globus v2 vs. Globus v4 vs. Glite etc)

Architecture Diagram



APAC Grid Operations Center

Test Date: Thu May 10 15:01:04 GMT 2007

[Home](#)

[APAC Grid](#)

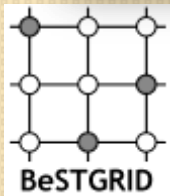
Menu

- [Gateway Status](#)
- [Usage](#)
- [Data Throughput](#)
- [Portal Status](#)
- [Help](#)

GITS Views

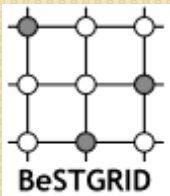
- [GITS Index](#)
- [ac3](#)
- [SAPAC](#)
- [QUT](#)
- [VPAC](#)

Hostname	Jobmanager	Ping	RSL-Hello	Hello World	Stage	RSL-Shell	Batch-Submit	Batch-Query	Batch-Cancel	Batch-Retrieve	GASS to remote site	GASS from remote site
ng1.sapac.edu.au	fork	Pass	Pass	Pass	Pass	Pass	Pass	Pass	Pass	Timed Out	Pass	Pass
ng1.sapac.edu.au	pbs:perseus@hydra	Pass	Fail	Fail	Fail	Not Tested	Pass	Pass	Fail	Fail	Fail	Not Tested
ng1.vpac.org	fork	Pass	Pass	Pass	Pass	Pass	Pass	Pass	Pass	Pass	Pass	Pass
ng1.vpac.org	pbs:sque@brecca-m	Pass	Pass	Pass	Pass	Not Tested	Pass	Pass	Pass	Pass	Pass	Not Tested
ng1.ivec.org	fork	Timed Out	Not Tested	Not Tested	Not Tested	Not Tested	Not Tested	Not Tested	Not Tested	Not Tested	Not Tested	Not Tested
ng1.ivec.org	pbs:express	Timed Out	Not Tested	Not Tested	Not Tested	Not Tested	Not Tested	Not Tested	Not Tested	Not Tested	Not Tested	Not Tested
ac.apac.edu.au	fork	Pass	Pass	Pass	Pass	Pass	Pass	Pass	Pass	Pass	Pass	Pass
ac.apac.edu.au	pbs	Pass	Pass with Warnings	Pass with Warnings	Pass with Warnings	Not Tested	Pass	Pass	Pass	Pass	Pass	Not Tested
ng1.hpcu.uq.edu.au	fork	Pass	Pass	Pass	Pass	Pass	Pass	Pass	Pass	Pass	Pass	Pass
ng1.hpcu.uq.edu.au	pbs:test	Pass	Pass	Pass	Pass	Not Tested	Pass	Pass	Pass	Pass	Pass	Not Tested



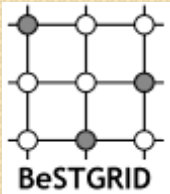
Grid Services (in VMs)

- A range of services are provided to support users of the grid, some of which run on the gateway servers and some of which run only at specific sites.
- Application support
 - Gridsphere Portals
 - Apache/tomcat
 - Authentication and Authorisation CA PKI and Shib via MyProxy/GRIDShib
 - Myproxy
 - AuthTool?
 - VOMS/VOMRS?
- Data Management
 - GridFTP sourced from VDT/globus
 - SRB
- Information Services
 - MDS2, MDS4 sourced from VDT/globus
 - GIIS
- Job Management
 - GRAM2, GRAM4 sourced from VDT/globus
 - Nimrod?
 - LCG (from EGEE)?
- Computers Servers run compatible PBS based schedulers and IBM Load Leveler
- Have clients for GridFTP and SRB installed to support remote data access



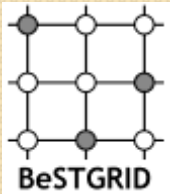
Adding a machine to the GRID

- user account
 - name: globus, UID: 646464
 - group: bestgrid, GID: 646464
- mount NFS directory from BeSTGRIDGATEWAY to /home/globus/.globus
- /etc/hosts: added IPs of BeSTGRIDGATEWAY
- iptables: added rules to accept tcp and udp protocols for BeSTGRIDGATEWAY
- pbs_mom:
 - installation directory: /opt/torque
 - client's binaries: /usr/local/bin/
 - pbs_mom binaries: /usr/local/sbin/
 - libraries: /usr/local/lib/
 - /etc/ld.so.conf: added /usr/local/lib
 - run pbs_mom under root account



Future

- Portals
- Linking in more systems to Grid
- Knowledge transfers to other NZ Universities and CRIs
- Beginnings of a National GRID framework
- Partnership with PRAGMA and EGEE
- Establish industrial links
 - NZSC (cluster)
 - Bio-industries (Biomatters, Cartesian GRIDspeed etc)



(for copies of this talk)

www.bestgrid.org

