Bio-grids and Applications

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Outline

- QFAB overview
- QFAB supplying data and tools for grids
- Case study

QFAB Overview

- Queensland Smart State grant of $1.9M under the National and International Research Alliances Program
- Matched by partners – total $3.8M
- Agreement to December 2009
- Collaboration of its partners, hosted at the University of Queensland

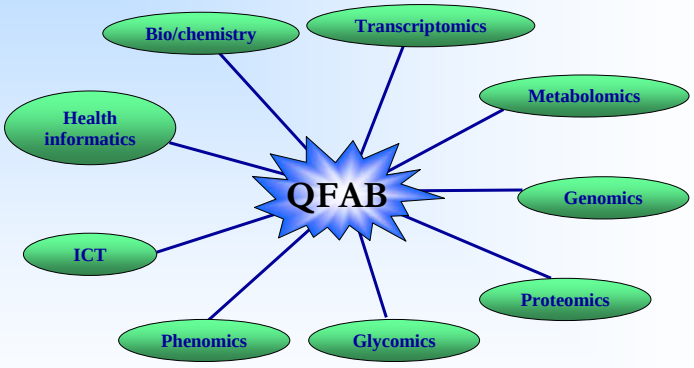
QFAB Vision

- To build a bioinformatics facility to deliver advanced solutions to support the biotechnology, ICT, research biology and clinical communities.

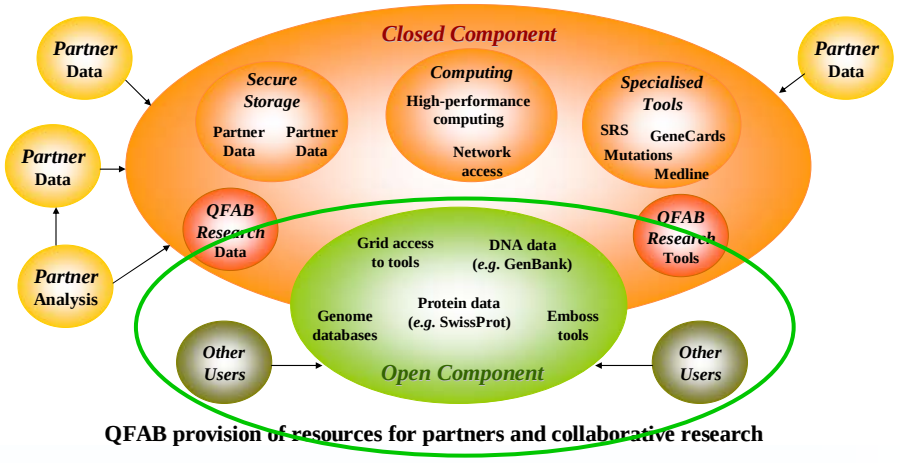
Partners

- Current
  - ARC Centre in Bioinformatics
  - e-Health Research Centre
  - SRC for Functional and Applied Genomics
  - Queensland University of Technology
  - Griffith University
  - Department of Primary Industries &Fisheries
  - Australian Partnership for Advanced Computing
  - Queensland Cyber Infrastructure Facility
- Future

Catalyst for multidisciplinary research



QFAB Operational Structure



QFAB provision of resources for partners and collaborative research

Grid Technology – our view

- Provides access to distributed data, information and services
  - large data collections in collaborative environments
  - compute intensive services
- Transparency of physical location and/or provider of resources
  - remote file operations where the user is unaware of where physical file is stored
  - access to one of many services offered by multiple suppliers

QFAB and Partners: enabling Bio -Grids

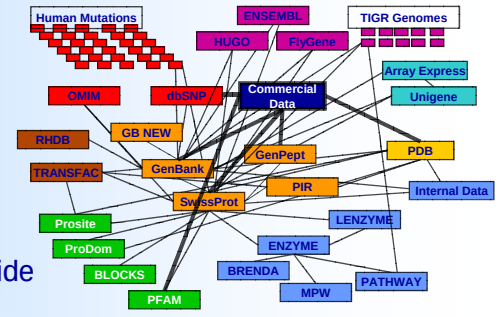
- Maintaining public domain data sets and tools
  - Automated updating of public datasets
- Making data available
  - Data put onto a grid with meta-data tags
- Integrating private and public data
  - Linking proprietary and public data without compromising IP ownership
- Providing web service interfaces to data and tools
  - Services for grids to access data (GENBANK, genome data) or to run compute intensive tools (BLAST, CLUSTAL)
- Workflow engines for using services

Computing and Storage

- In-house
  - Secure cluster available for partner projects
- QCIF and APAC
  - Use of QCIF and APAC high performance computing for running analyses and indexing data
- APAC Grid
  - QFAB will contribute data and tools to the APAC grid program

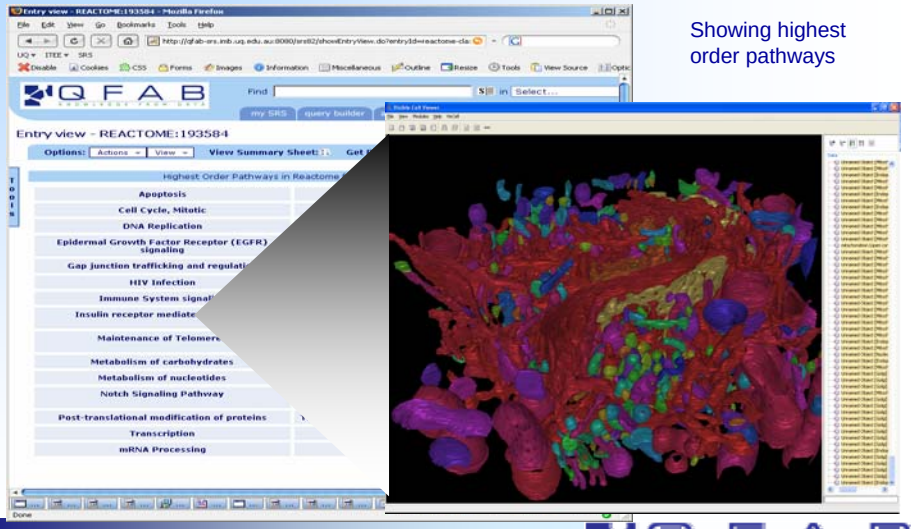
What is QFAB making available to the grid?

SRS



- Commercial tool used extensively in the pharma and biotech industries worldwide
- Integrates partner data with public data
- Over 1000 different data sets available for inclusion
- Feature packed web browser for quickly searching and viewing data
- Analysis tools available, with links to public data
- Automated updating of public data
- Web services interfaces for building custom applications

Reactome for Visible Cell™

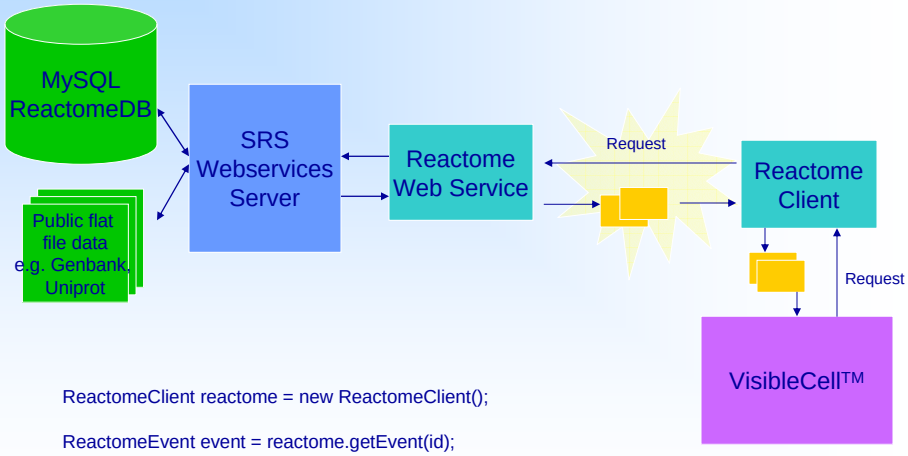


Showing highest order pathways

Reactome for VisibleCell™

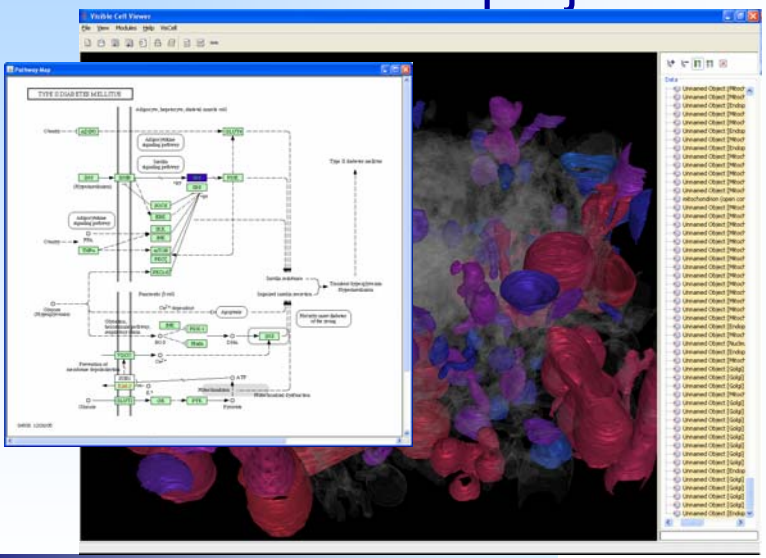
- Integrates
  - Reactome
    - pathway,
    - reaction,
    - gene ontology (GO) data
  - Visualiser interface of the ACB VisbleCell™ project

Reactome Web Service




```
ReactomeClient reactome = new ReactomeClient();

ReactomeEvent event = reactome.getEvent(id);
ReactomeComponents[] components = reactome.getComponents(id);
```


ACB VisibleCell™ project



Storage Resource Broker (SRB) at QFAB

- Data grid for sharing data on an international scale
- Provides user with a single file hierarchy for data distributed across multiple storage systems
- At QFAB since March 2007
  - Currently at IMB and Griffith University
- Communication to more nodes planned

Storage Resource Broker (SRB) at QFAB

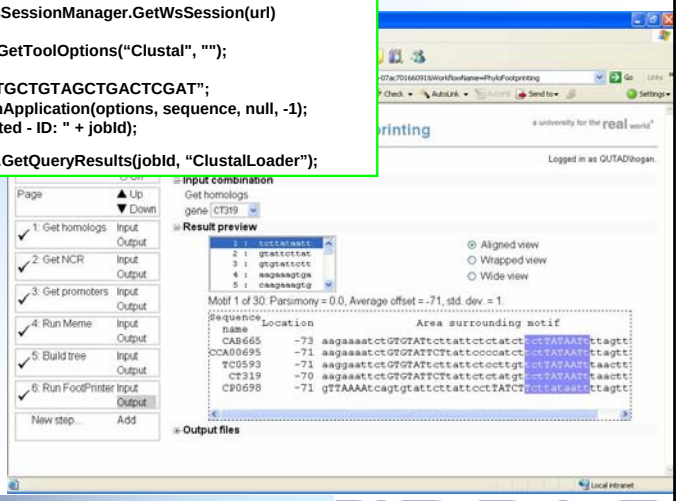
- Maintain up-to-date copies of public data in SRB
  - Data sets: GENBANK, GO, PDB, UNIPROT etc
  - SRS updates data and automatically executes command to update SRB and make files available
    - Next step: Automatically add meta data to files
- UCSC and ENSEMBL genome datasets
- More data sets can be added as requested

GPFlow: Bioinformatics workflows

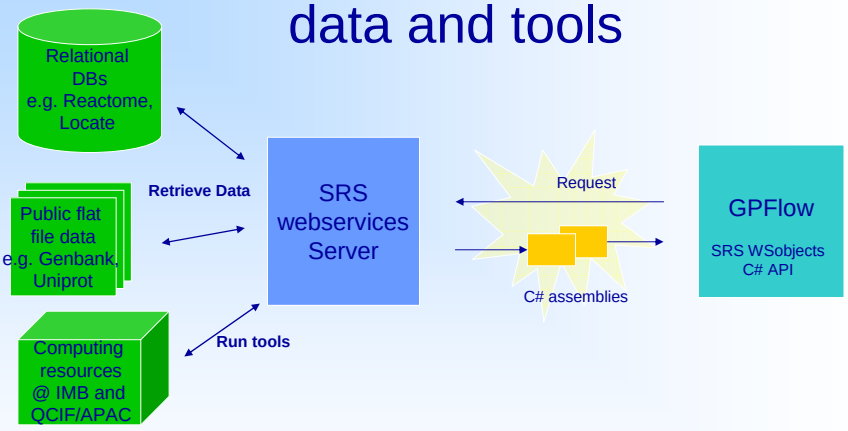
- QUT Workflow engine technology
  - Builds and runs bioinformatics workflows for in-silico genomics experiments
  - Designed to meet the scientists at the bench without the need to write code
  - Interactive and immediate
  - Built on Microsoft business technology

GPFlow – no code required

```
WsSessionImpl wsSession = WsSessionManager.GetWsSession(url)

SrsObject options = wsSession.GetToolOptions("Clustal", "");

String sequence = "CGATCTGATGCTGTAGCTGACTCGAT";
string jobId = wsSession.LaunchApplication(options, sequence, null, -1);
Console.WriteLine("Job Completed - ID: " + jobId);

SrsObject[] results = wsSession.GetQueryResults(jobId, "ClustalLoader");
```



GPFlow accessing QFAB data and tools



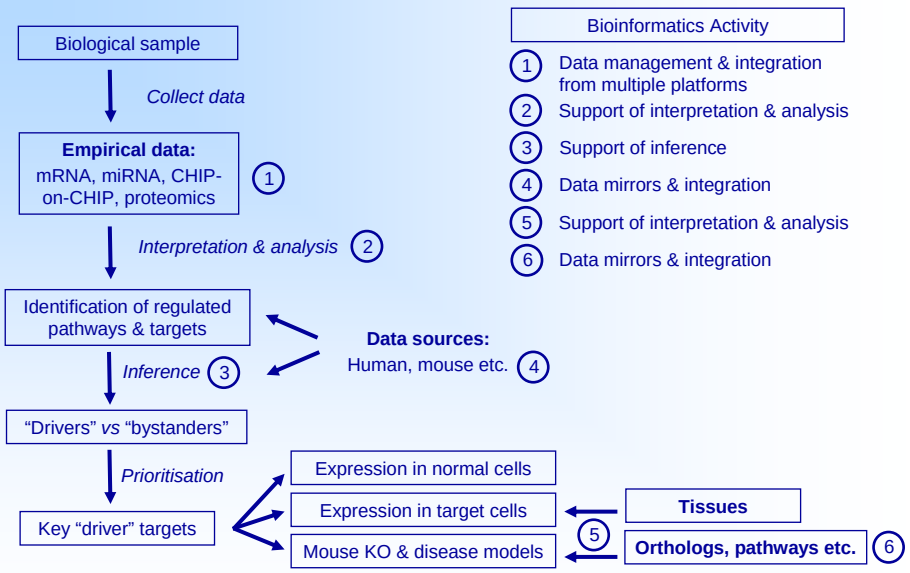
Bringing it Together

Case Study

- Using bioinformatics to underpin a research partnership to identify a regulatory pathway important in a specific cancer and hence identify targets
  - Researchers wish to identify all sources of information about a particular cancer
  - link these to clinical and experimental data to develop a validated model of action
  - ultimately identify key drivers which may lead to drug targets.

Key steps and challenges

- Identify sources of information about the cancer, including patient data
- Link to and integrate known data sources – genomic, proteomic, biomedical imaging, chemoinformatic, molecular modelling
- Develop model pathways and mode of action
- Test experimentally
- Validate model
- Identify key drivers and influences



QFAB meeting these needs

- Portal to provide researchers with access to data
  - Federated data from SRB
  - Tools to import data from dispersed technology platforms e.g. linking into the DART/ARCHER project at Monash
- Secure data storage and access, authentication protocols
- Develop ontology to enable reasoning across data sources
- Data integration tools
  - SRS for public datasets
  - HDI for private clinical data integration
- Providing or linking with data analysis tools for model development, testing and validating
- APAC and QCIF Computing power

Bio-grid and QFAB applications

- QFAB is making data and tools available for grids to use:
  - Data already available via SRB grid applications
  - SOAP based services available for inclusion into Grids
- Underpins large collaborative research projects asking the big questions

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