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KidneyGrid: A Grid Platform for Integration of Distributed Kidney Models and Resources

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Outline

- Introduction
- What is KidneyGrid
- Design and Implementation
- Evaluation
- Live Demo
- Conclusion and Future work

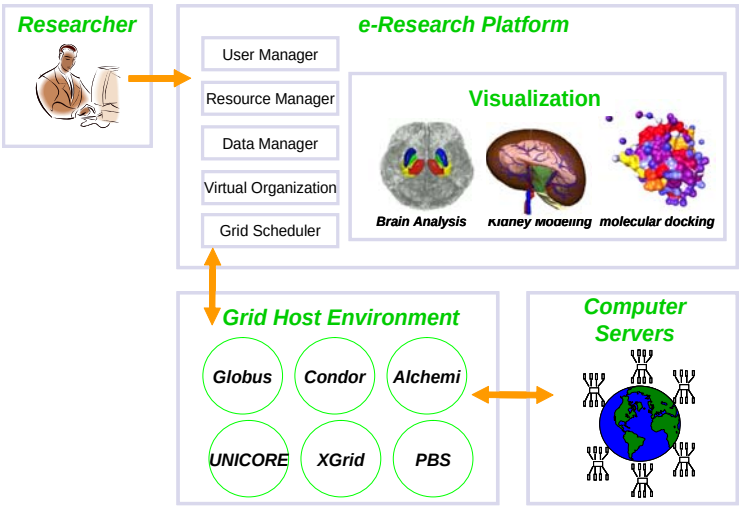
Introduction

- Mathematical modeling has been used successfully in analyzing the huge volume of biomedical data
  - Such as modeling heart physiology, lung physiology, kidney physiology
- Many models exist
  - Various formats
  - Various simulation environments
- Generally proprietary and incompatible
  - Extremely difficult to access and integrate various models and resources
- Various legacy kidney models and resources
  - Different implementation techniques such as command line, graphical interface

Grid computing in e-Research

- Grid computing provides
  - Powerful computation facilities (means researchers can run their existing research faster)
  - Other facilities such as working in collaborative environments, reducing costs, and gaining access to an increased number of resources and instruments

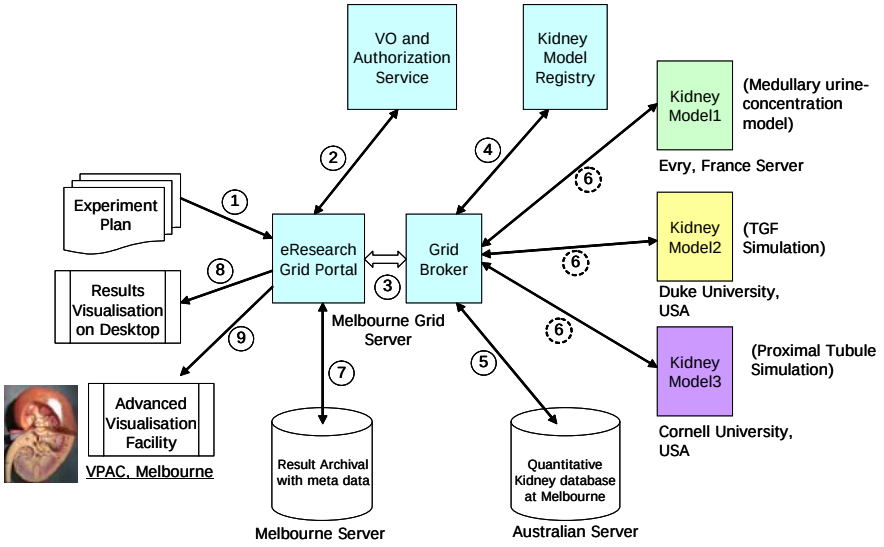
A typical e-Research vision



What is KidneyGrid?

- An ARC e-Research Project developing a Grid platform for access to distributed kidney models and resources including
  - an interactive web interface to a collection of distributed legacy models
  - a way to plan, execute and monitor the experiment over grid resources
  - and a kidney virtualization to better present the outcome of the experiment
- Part of the larger Physiome Project
  - An internationally collaborative open source project to provide a public domain framework for computational physiology

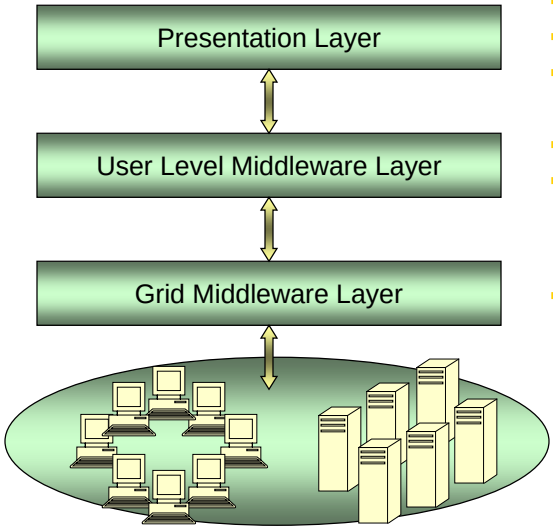
System Architecture



Issues to be addressed

- Standard
  - a platform for ‘plug and play’ modeling
  - a standard basis of representation for all models and their data
- Interoperability
  - Sufficient legacy kidney models for the site to be opened to the general community
  - Integration of various legacy application written by different programming language

Technology choices



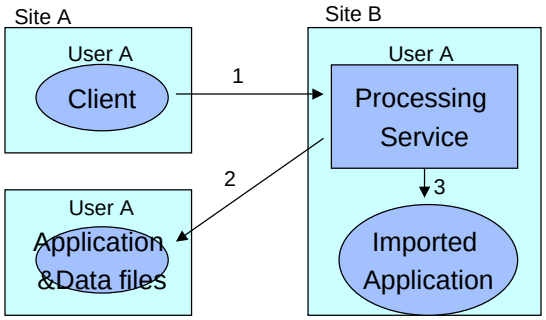
- Gridsphere Framework
- Java Server Faces
- Java Applet
- Gridbus Broker
- Web Service Resource Framework (WSRF)
- Globus & Alchemi
- Work Station, Server or Cluster

Web Portal Development

- User interface for the researchers
- Utilize Gridsphere Framework
  - open source and JSR 168 (Java portlet standard) compliant
  - Reusable modules such as user management
  - mature and widely used by other grid portal related projects

Legacy Application Integration Model (Explicit Model)

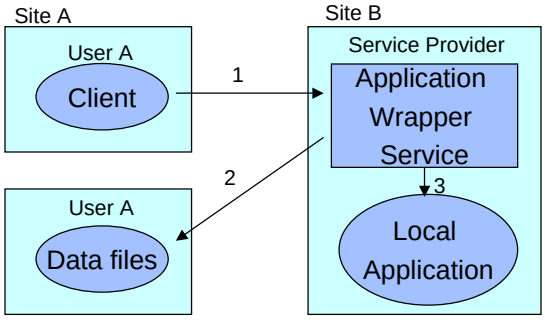
- Explicit Model (typical of GT-2) (J. Giddy et. al, 2005)



  - User explicitly specifies the resources, executable program, program's arguments and environment, and data files. User takes full responsibility to update it

Legacy Application Integration Model (Wrapper Model)

- Wrapper Model (Web Services based) (J. Giddy et. al , 2005)



  - Application is hide to user to avoid dependencies between client and service provider
  - User don't need an account on the site running the application
  - Authorization to use the service can be controlled by the service provider

Legacy Application Integration

- Avoid dependencies on the legacy application
  - Need a generic way to communicate with various models
- Adopt the wrapper model for integration
  - Implement a service wrapper for each models
- Utilize the Web Service Resource Framework (WSRF)
  - It is stateful (useful for long running simulation)
  - Can be deployed into globus container (make each model a grid service)
  - Support Windows Platform via WSRF.net and Alchemi
- For each service wrapper, we implement
  - A WS-Resource for each model representing possible state such as parameters or simulation status
  - A WS-Notification mechanism for long running simulation

Grid Resource Broker

- Gridbus Broker is a user-level middleware
  - Easy to use
    - Pure Java-Based, Open Source, Well-Documented
    - Services including application composition, scheduling, monitoring, result collection and QoS
  - Flexible and Extensible
    - Higher level abstraction for various low level grid middleware such as globus, unicore, achemi etc.
  - Scalable
    - Least State: stateful information are stored in DB other than memory
    - WSRF interface for the Broker: can be deployed as web services

Experiment Plan and Execution

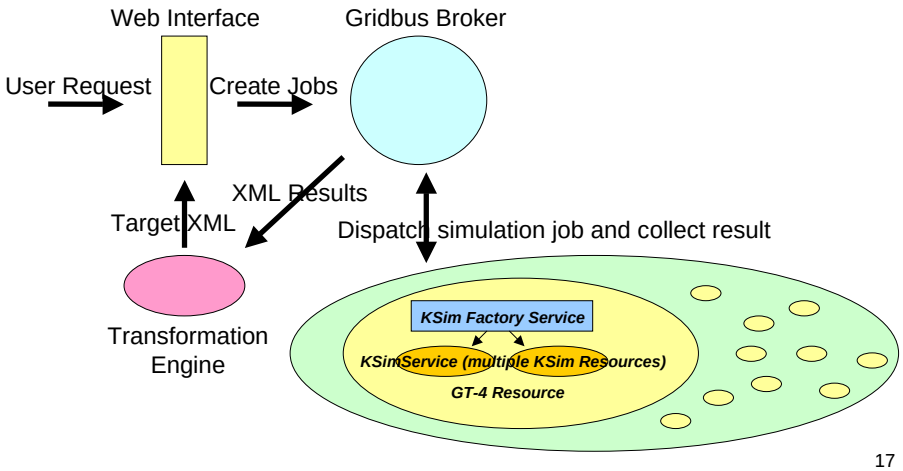
- Prepare the experiment by modifying the parameters via web pages
- Submit the experiment plan to the Gridbus Broker
- Execute simulation on remote grid resources via the service wrapper
- Monitor the execution of the experiment

Visualization

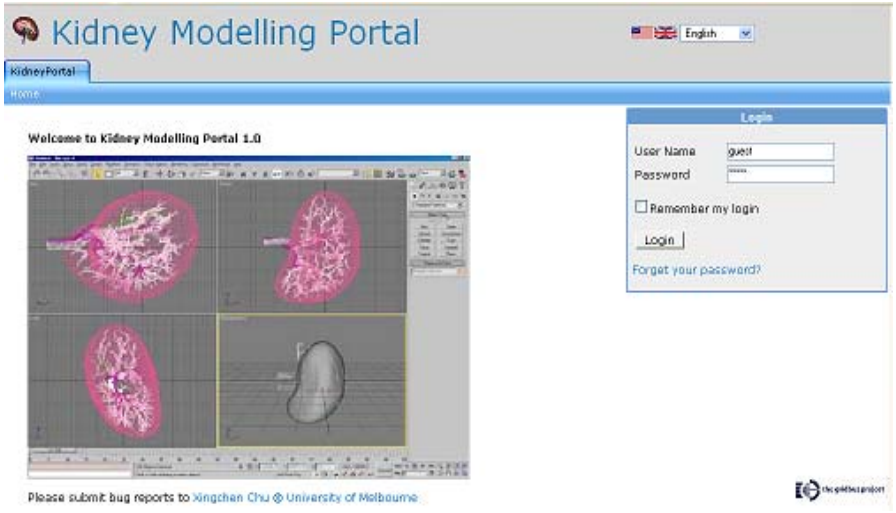
- Need to generic visualization facility to demonstrate all the models
- Require a standard format to represent the underlining data (XML schema)
- Transformation from various results into the standard data format
  - Utilize XSLT transformation (provide a stylesheet for each kidney model), not be able to handle non-xml format data
  - Other transformation technique for non-xml format data

Evaluation

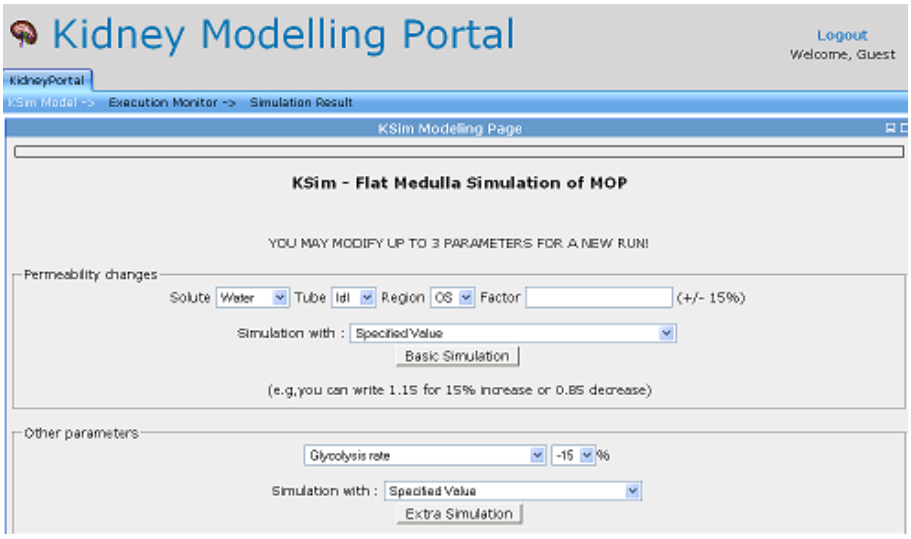
- An integrated kidney model called KSim (written by fortune language)



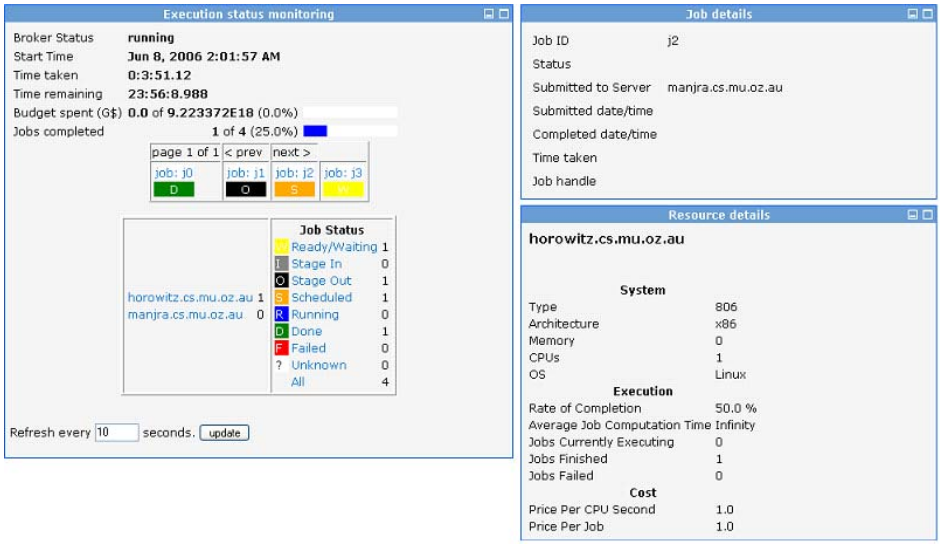
Portal Snapshot (I)



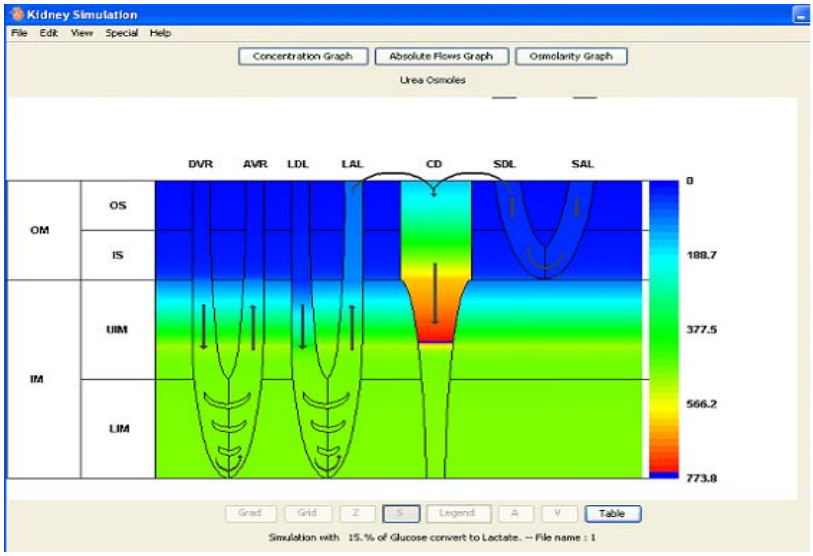
Portal Snapshot (II)



Portal Snapshot (III)



Portal Snapshot (IV)



Experiment (I)

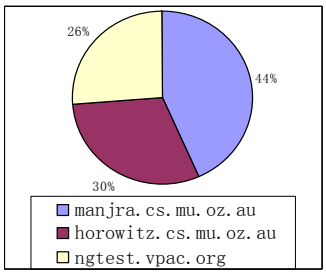
- The possible simulation cases for KSim

$$T = C_s^1 \times C_t^1 \times C_r^1 \times C_{fn}^1 + C_x^1 \times C_{fx}^1$$

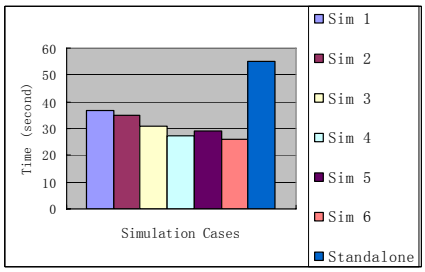
  - T is the total number of cases, s (5), t (7), r (4), x (3) stand for solute, tube, region and extra parameter respectively, fn (3) and fx (31) are the acceptable factor for basic and extra simulation
  - The total number is then 513

Experiment (II)

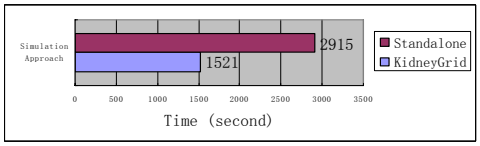
- We tested 53 cases on 3 grid resources



(a) Job Completion Rate



(b) Average Job Execution Time



(c) Total Job Execution Time

Advantages of the KidneyGrid

- Scalable
  - Separate the portal process and Gridbus broker process into different JVM increase both the scalability and performance of the system
  - we achieve this utilizing the new WSRF interface for Gridbus Broker
- Secure
  - The wrapper model for integrating legacy application enhance the security
  - The service provider controls the service they want to provide to the users
  - Users won't need to upload the executable program to the grid resource which may generate security concerns
- Extensible
  - Easy to extend to support other kidney models once required
- Heterogeneous
  - Support diversity of kidney models and resources

Live Demo

Conclusion and Future Work

- A grid platform for distributed kidney models has been developed
  - Experiment plan, execution, monitoring and visualization
  - Integration of the legacy application (KSim) into system based on web services
- Integration of more legacy kidney models
- Transformation for each model to a generic visualization tool
- Implementing VO-based scheduling, resource discovery and management.

Thanks for your attention!

We Welcome Cooperation in Research and Commercialisation!
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Reference

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- L. Zhou, A. Matsunaga, V. Sanjeepan, H. Lam and J. A. B. Fortes, *Application Modelling and Representation for Automatice Grid-Enabling of Legacy Applications*, Proceedings of the e-Science 2005, Dec. 5-8, 2005, Melbourne, Australia.

Technology choices

Component	*Technology Used*	*Comments*
Portal	Gridsphere Framework	Reusable web components. JSR 168 portlet standard compliant. Open source and widely used for grid portal development.
Virtual Organization	MyProxy	Only consider the authentication for the VO, may extend to completed VO system such as VOMS
Grid Resource Broker	Gridbus Broker V3.0	Provide ability to support Web Service Resource Framework (WSRF), various scheduling algorithms and resources such as globus and alchemi
Service Wrapper for Legacy Kidney Model	Web Service Resource Framework (WSRF)	WSRF provides stateful web service which is able to deployed on the globus toolkit 4 (gt-4) container
Visualization	VPAC Advanced Visualization Facility in Melbourne	Provide Java Applet that can be easily integrated into web portals
Core Grid Middleware	Globus Toolkit 4, Alchemi, UNICORE	Provide supports for integration of grid resources accessible through low level grid middlewares