Agenda

- Project Overview
- What is a VRE?
- What is Integrative Biology?
- Requirements for a VRE
- IBVRE Infrastructure
- Development Plan
Project Overview

- JISC funded project running for 2 years
- Part of a wider VRE Programme.
- One of three Oxford VRE projects, others being:
  - Building a VRE for the Humanities (BVREH)
    - led by Humanities Division, University of Oxford
  - Sakai VRE Demonstrator
    - collab. with Lancaster University (lead), CCLRC, and Portsmouth University
• Project Team:
  – Matthew Dovey (OUCS) – Project Director
  – David Gavaghan (ComLab) – PI
  – Andrew Simpson (ComLab) – PI
  – Matthew Mascord (OUCS) – Project Manager
  – Clint Sieunarine (ComLab) – Developer – User Interface
  – Geoff Williams (ComLab) – Developer – Systems

• Consultant:
  – Marina Jirotka (ComLab) – Requirements
What is a VRE?

• VRE stands for “Virtual Research Environment”

• Original idea was:
  – Research analogue of the VLE (Virtual Learning Environment)

• Working definition:
  – Framework
  – Collaborative Tools
  – Support for Research Processes
What is Integrative Biology?

• EPSRC e-Science Pilot Project – budget ~ £2.4M
• International consortium of heart and cancer modelling groups led by Oxford University
• Tackling heart disease and cancer through:
  • Science
    • large-scale (multi-scale) computer simulations of biological behaviour – *in silico* experiments
  • Technology
    • construction of a Grid infrastructure supporting this community giving tailored access to Grid resources e.g. NGS, HPCx. CSAR, SRB.
Heart vs Cancer Modelling

**Heart:**
- Globally distributed
- Established (30 years)
- Computational Biology (lets build something)
- Computer based
- Running large-scale simulations to increase understanding of the biology – in silico experiments

**Cancer:**
- UK-based
- Relatively New
- Mathematical Biology (lets analyse it)
- Pen and paper based
- Running small-scale simulations to refine the models
Integrative Biology VRE

• To extend support to the entire research “life cycle”, the wider context within which the research is conducted:
  – Identification of research idea through to dissemination and provision of training.
• To form the recognised front-end to the IB Grid infrastructure – replacing existing IB portal.
• Focus on web portal technologies: JSR-168 (Java Portlets Standard), WSRP (Web Services for Remote Portlets)
IBVRE Infrastructure – VRE Architecture

[Diagram showing the architecture of the IBVRE Infrastructure with layers: Presentation layer, Front end layer, Business logic layer, Resource layer, showing interactions and components such as Mathematical Modelling Tools (Matlab), IB Workbench (myGrid), VRE Framework, WSRP, WSRP-PRF, Resource Directory, WebService API, Data Resource, Compute Resource, IB Middleware, and Other VRE Tools: Real Time Communication, Blogs, Calendars, Etc.]
IBVRE – Work to date

- Has focussed on two main work packages:
  - Workpackage 2 – Research Process Analysis (Clint, Marina, Matthew)
  - Workpackage 3 – IBVRE Infrastructure (Geoff)
    - Project Management Environment
    - Portal Infrastructure
What are the requirements for an IB VRE?

• Three-month qualitative (scoping) study carried out
  – One to one interviews
  – Focus group
• Eleven researchers participated, representing nine of the consortium’s research groups.
• Initial analysis report published November 2005 (available on website http://www.vre.ox.ac.uk/ibvre).
Requirements – Typical Interview

- Open-ended and un-structured
- Recorded with permission
- Typical day
  - higher level research lifecycle
  - scientific workflow
  - activities unrelated to core science e.g. lab meetings
  - artifacts used e.g. lab books, postits, todo lists
Requirements – Focus on Collaboration

• For each activity
  – How is knowledge divided across the actors in the collaboration, who does what?
  – How time critical is it - synchronous or asynchronous?
  – Distributed or co-located?
  – Is it confidential – public or private?
  – Do you need to see the other person?
  – What technologies are used?
Requirements – Post Interview

- Research process is written up and signed-off by the interviewee
- Follow-up sessions arranged where necessary
Requirements – Focus Group

- Piggy-backed onto IB project workshop 2005 (breakout session)
- Recorded and transcribed
- Similar scope to interviews
- Aim to obtaining consensus on a priority
Requirements – Key Findings

• Day-to-day support critical
• Heart modelling
  – management of in silico experimental process
  – collaborative visualisation
  – capturing collaborative discussions
  – linking experiments to wider context
• Cancer modelling
  – management of paper-based notes
  – transfer of best practice
In silico experiments

1. identifying models
2. identifying or developing efficient algorithms
3. developing the core simulation codes – C++ or Fortran
4. for each in silico experiment:
   a. developing scripts
   b. running the simulation(s)
   c. downloading data
   d. generating figures – movies, graphs
   e. discussing the figures

• Varying experimental practices + difficulties with software tools imply reproducibility problems.
• Vision is to capture everything needed to reproduce an experiment trivially.
• Can potentially aid the training of new researchers.
Mathematical Modelling

• Mathematical modelling carried out through face to face discussions with experimentalists in front of a whiteboard.

• Subsequent analytical work
  – Done individually
  – Paper and pen-based
  – Intermittent use of MatLab/Maple to obtain quick answers and to run small-scale simulations.
  – Important results LaTeXed up into papers
  – All other preliminary work filed in filing cabinets.
VRE Infrastructure

- Procurement and installation of project and test servers
- Portal Framework
  - Initial uPortal 2.5, moving to uPortal 3 when stable
- Project Management Server:
  - Trac
  - Subversion
  - Continuous Integration Framework
- Initial design report available on project website
Development Plan

- Re-branded IB portal VRE release at the end of February
- Focus on high priority requirements only
- Bespoke development:
  - In silico experiment + research context repository
- Detailed requirements/prototyping work:
  - Dr James Easons Virtual Heart Lab, Washington and Lee University (February)
  - Prof Natalia Trayanova’s Lab, Tulane University (March)
- Third-party technology evaluation:
  - Anoto Paper
  - Vannotea
Thank you

• Project web site and reports:
  – http://www.vre.ox.ac.uk/ibvre

• Questions?