The Integrative Biology VRE Project

*OeRC Seminar, 13 October 2006*

Berners-Lee Room, Oxford University Computing Services

Matthew Mascord, Project Manager, Oxford University
Overview - Integrative Biology

- IB is an EPSRC-funded e-Science project tackling UK’s two biggest killers: cancer and heart disease through large-scale multi-scale simulations.

- Globally distributed and interdisciplinary community: US, Europe, New Zealand

- Developing a web-services based grid infrastructure providing tailored access to compute and data resources.
Overview - IBVRE

- 2-year project funded by JISC (UK Joint Information Systems Committee), based at Oxford, started April 05
- Developing a Virtual Research Environment for the IB research consortium.
- To form the recognised visual gateway to underlying IB services (the IBVRE portal).
- Address needs not originally within the IB remit:
  - Supporting collaboration
  - Supporting the full research lifecycle
Team

- **PIs**
  - Professor David Gavaghan, Project Director (Computing Laboratory)
  - Dr Andrew Simpson (Computing Laboratory)
  - Dr Michael Fraser (Computing Services)

- **Core Staff**
  - Matthew Mascord, Project Manager (Computing Services)
  - Geoff Williams, Developer – Systems (Computing Laboratory)
  - Clint Sieunarine, Developer – User Interface (Computing Laboratory)
  - Michael Loizou, System Administrator (Computing Services)

- **IB Liaison**
  - Damian Mac Randal, Technical (CCLRC)
  - Sharon Lloyd, Management (Computing Laboratory)

- **Consultants:**
  - Dr Marina Jirotka, Requirements (Computing Laboratory)
  - Andrew Foster, Technical (Computing Services)
Initial work

- Two parallel strands:
  - IBVRE Infrastructure (Geoff Williams)
    - Project management environment based on Trac
    - VRE portal infrastructure
  - Research Process Analysis (Matthew Mascord, Marina Jirotka, Clint Sieunarine)
Initial work - development

- Migration of existing IB prototype portal to a production environment
- Based on uPortal 2.5
- uPortal chosen because:
  - Community movement and support
  - In-house (Oxford) experience
- Develop new look and feel.
- Hosting existing IB portlet tools.
Initial work – analysis (1)

- Three-month qualitative (scoping) study carried out
  - One to one interviews
  - Focus group
- Eleven researchers participated, representing nine of the consortium’s research groups.
- Open-ended, un-structured, recorded.
- Focus group transcribed, aimed to establish priorities
- Priority should be day-to-day support.
## Initial work – analysis (2)

<table>
<thead>
<tr>
<th>#</th>
<th>Requirement</th>
<th>Heart/Cancer</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Tool to assist management of the in silico experimental process.</td>
<td>Heart</td>
<td>Development</td>
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<tr>
<td>3.</td>
<td>Tool to provide notification of biological journal papers.</td>
<td>Cancer</td>
<td>Evaluation of Subject Portals Project Tools (ILRT)</td>
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<tr>
<td>4.</td>
<td>Tool to facilitate collaborative visualisation</td>
<td>Heart</td>
<td>Vannotea Evaluation (University of Queensland)</td>
</tr>
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Digital Paper
Digital Paper

- Logitech IO2 digital pens being evaluated with 11 heart and cancer modellers.
- To investigate the extent to which the technology can help scientists manage their paper-based material and define the requirements for future development.
- Main scenarios:
  - Heart - replacement for lab books.
  - Cancer - replacement for paper used for mathematical modelling.
Digital Paper - Technology

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Digital Paper - Evaluation

- Methodology:
  - Diary study
  - Mini-workshop at the IB Project Workshop 2006 inviting...
    - Participants in the evaluation
    - Invited other experts in this area
  - Follow-up interviews

- Reporting back to
  - Academic community
  - Digital pen manufacturers
Digital Paper – Usage Scenarios

- **Some Uses**
  - In conjunction with email
  - Supervisions
  - Note-taking
  - Experiments
  - Mathematical modelling
  - Laboratory Notebook
  - Mathematical presentation

- **CERN (Francois Grey)**
  - OpenLogBook

- **PaperWorks, KCL (Paul Luff)**
  - Augmented textbook (Pearson), museum activity sheets, bespoke guidebook, auction catalogues, new ways of giving presentations
Positives and Negatives

+ve:
- nice to have the backup
- great for emails
- integration with google desktop
- tablet has more functionality but pen good when tablet cumbersome
- pen size good
- output good

-ve:
- Spidering problem
- CPU Usage + performance
- OCR not as good as tablet
- pressure sensitivity
- problems with greek, chemical names and tabular columns
- no linux/mac solution
- cost concerns – scrap often used for maths

(Many problem with the logitech pens implementation not the technology itself)
In silico experiment repository
In silico experiment repository

- To provide an interface allowing
  - Experiments to be designed and executed entirely through a visual interface without the need to use the command line.
  - The results from past experiments to be retrieved and trivially reproduced.
- Meet specific needs first, to prove the concept, generalise later.
- Design workshops at two heart modelling labs in the US:
  - Dr James Eason’s lab at Washington and Lee University (WLU), Virginia (Jan 06)
  - Professor Natalia Trayanova’s lab at Tulane University, New Orleans (May and Jul 06)
Workflows, myGrid, and Taverna

- Taverna (myGrid) provides for the visual composition of data-driven workflows.
- Linux or Windows client – not currently web/portal based.
- Main user community is the bioinformatics community, to mine existing data sets.
- By contrast, IB is generating data *in silico*.
- Workflows difficult to break-down (usually dominated by single executable)
- Lots of parameter sweeps – Taverna doesn’t really support this (yet).
- Data usually flows straight into viz packages, less processing.
- At this stage benefits don’t justify cost.
- VRE project focusing on the interface.
WLU and Tulane

- **WLU:**
  - Targeted set of experiments
  - 4th year undergraduates (often biology majors) help with the execution of pre-designed experiments
  - Clear need for a VRE

- **Tulane:**
  - greater diversity of experiments
  - each lab member designs and executes their own experiments
  - harder to see the need for a VRE (members proficient at scripting)

- **Potential Benefits:**
  - reducing the ramp-up time for new lab members, and
  - make it easier for simulations to be reproduced by others.
  - off-screen visualisation rendering to check status and produce videos or stills for sharing.
  - standardise the organisation of parameter searches.
Research process storyboarding at WLU

Divided experiment up into chunks
WLU Experiments

- Components:
  - Geometry Model (e.g. Rabbit, Canine, Human etc)
  - Membrane Dynamics (e.g. Luo Rudy)
  - Electrical Parameters (e.g. Conductivity, Capacitance)
  - Tissue Properties (e.g. normal, ischemic, infarct)
  - Initial Conditions (e.g. systole, diastole, reentry)
  - Stimulation Protocol (e.g. shock/pacing/mechanical)
  - Numerical Parameters
  - Software/Hardware Version
  - Post Processing (e.g. success/failure, ECG, movies)
  - Storage

- Found only a handful are routinely modified by experimentalists.
Analysis of an individual’s process at WLU

- Video observation of an individual scientific workflow at WLU
- Revealed the intricate nature of the process
- Helped identify what needs to be reproduced in the VRE
User interface design at WLU (1)

- Sketched out tailored interface for Vulnerability Grid experiments
  - Experiments that test the affect of timing and strength of a shock applied to a simulated ventricle.
- Would work for a majority of simulations performed at the lab.
User Interface Design at WLU (2)

- **Experiment**
  - Min & Max Strength
  - Min & Max Time
  - Tilt
  - dt1, dt2
  - Epsilon
  - Waveform
  - Duration

- **Batch**
  - Min & Max Strength
  - Strength Increment
  - Min & Max Time
  - Time Increment

- **Shock**
  - Strength
  - Time
User interface design at WLU (3)
WLU UI Evaluation

- Evaluated with both an experienced and new student.
Design Workshop at Tulane University

- Similar exercise at Tulane.
- Greater range of experiments.
- More generic solution required.
- Generic way to do parameter searches.
UI Design at Tulane (1)

- Killer feature is off-screen visualisation rendering, exposed through the VRE.
- 6-way snapshot showing surface electrical activity.
- Generation of movies and stills from completed experiments.
UI Design at Tulane (2)
Subsequent Development (1)

- Designed an interface bridging the requirements of the two groups.
- Initially building standalone applications for the two labs.
  - Linking to local computational resources
  - Standard web application
  - Concept proving
- Planning to implement Autumn/Winter 2006.
- Next steps are to
  - “Portalize”
  - Link fully into IB web services infrastructure giving seamless access to SRB, NGS and HPCx.
Subsequent Development (2)
Thank You!

Project Website:
http://www.vre.ox.ac.uk/ibvre

VRE Portal:
https://vre.integrativebiology.ac.uk/

Questions?