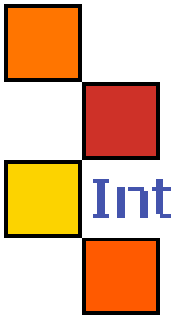


IBVRE

Integrative Biology Virtual Research Environment

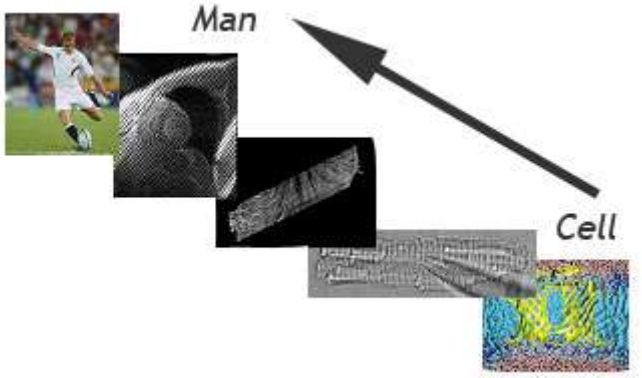
The Integrative Biology VRE Project

User Requirements Gathering for the Humanities
Workshop Two – Requirements Gathering in eScience

Oxford University Computing Laboratory
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 inter-disciplinary 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

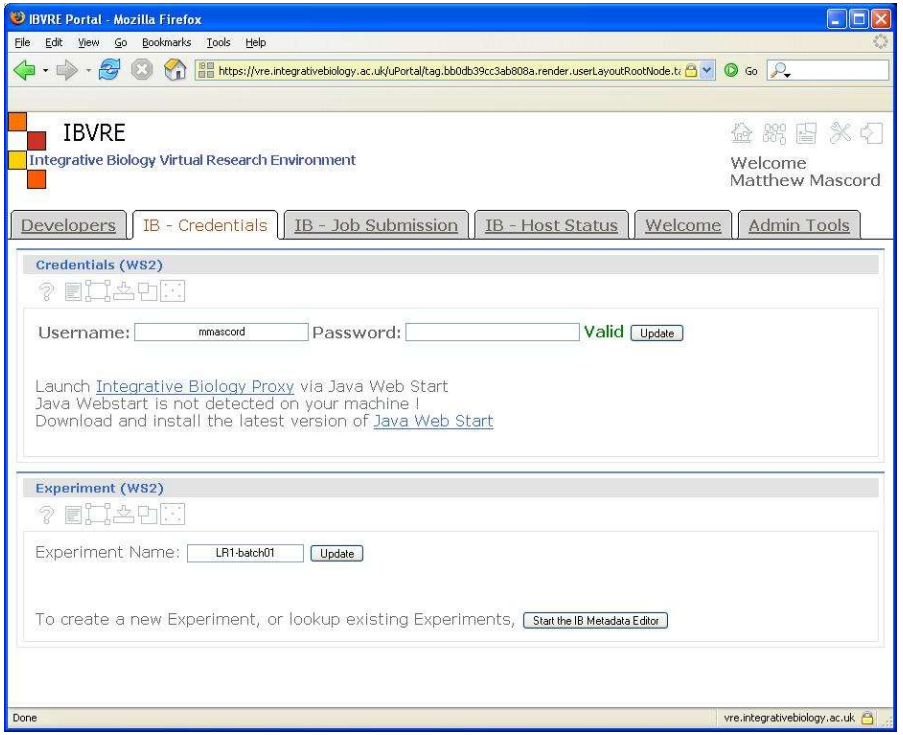
- PIs
  - Professor David Gavaghan, Project Director (Computing Laboratory)
  - Dr Andrew Simpson (Computing Laboratory)
  - Dr Michael Fraser (Computing Services)
- Core Staff
  - Matthew Mascord, Project Manager (Computing Services)
  - Geoff Williams, Developer – Systems (Computing Laboratory)
  - 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)

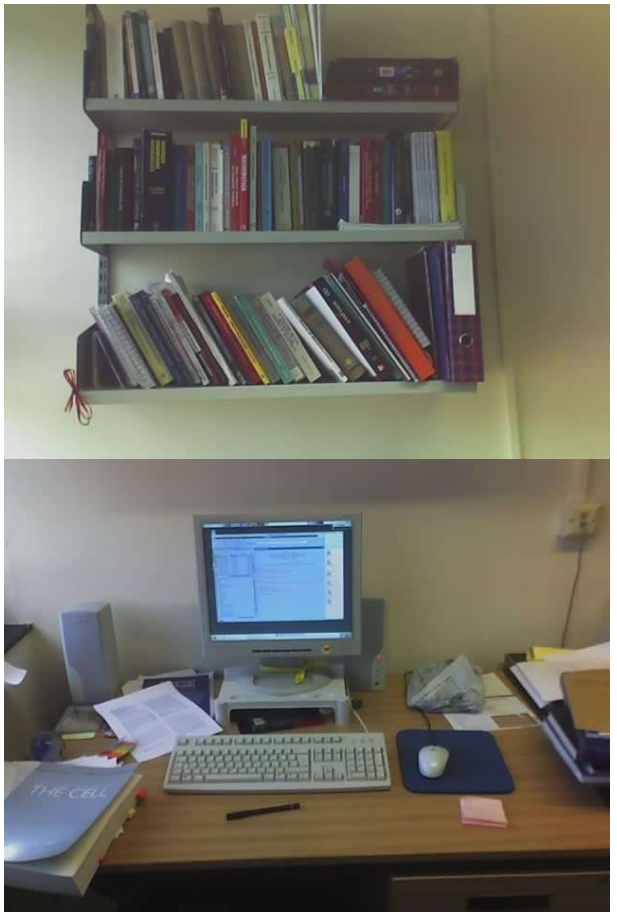
Initial work - development

- 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)

#	**Requirement**	**Heart/Cancer**	**Method**
1.	Tool to assist management of the in silico experimental process.	Heart	Development
2.	Tool to manage paper-based material.	Cancer, Heart	Digital paper evaluation.
3.	Tool to provide notification of biological journal papers.	Cancer	Development & Jafer Portlet Evaluation
4.	Tool to facilitate collaborative visualisation	Heart	Vannotea Evaluation

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)

WLU and Tulane

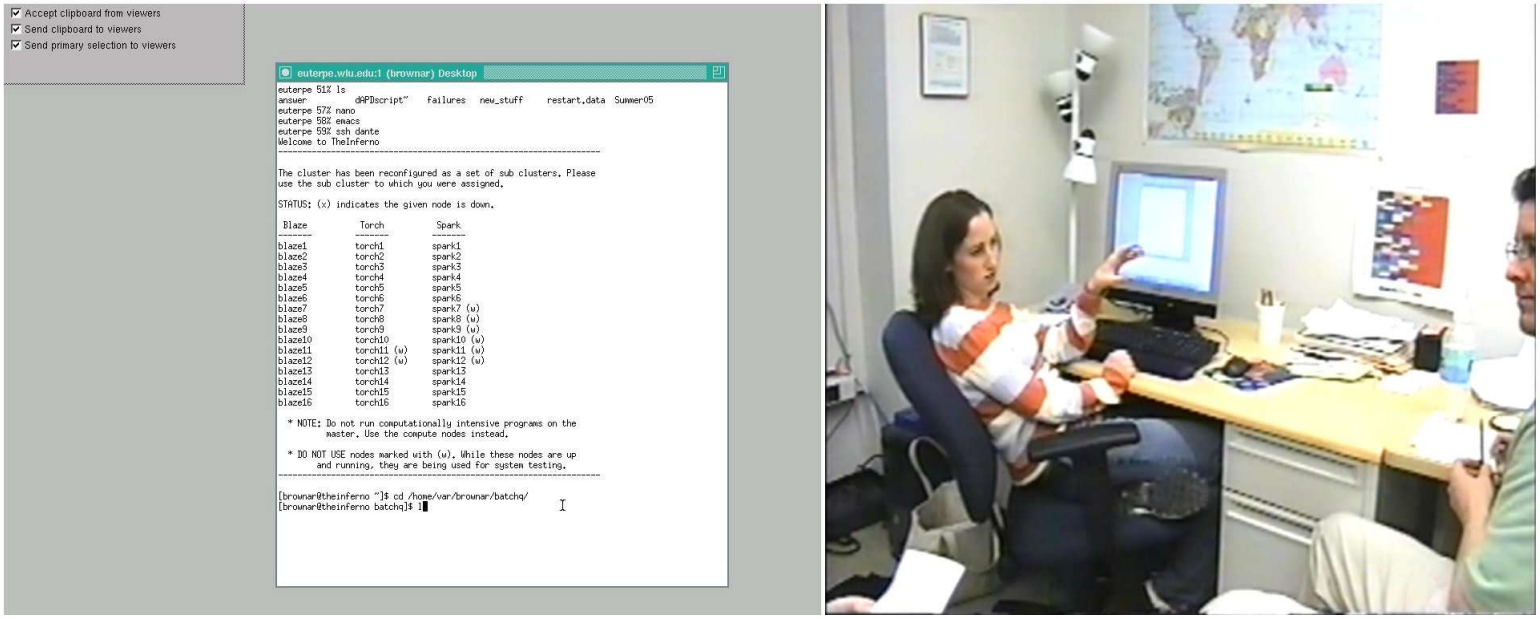
- WLU:
  - Targeted set of experiments
  - 4th year undergraduates (often biology majors) help with the execution of pre-designed experiments
  - Clear need for a VRE
- Tulane:
  - greater diversity of experiments
  - each lab member designs and executes their own experiments
  - harder to see the need 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.

Only a small number of parameters are modified across experiments.

Analysis of an individual's process at WLU

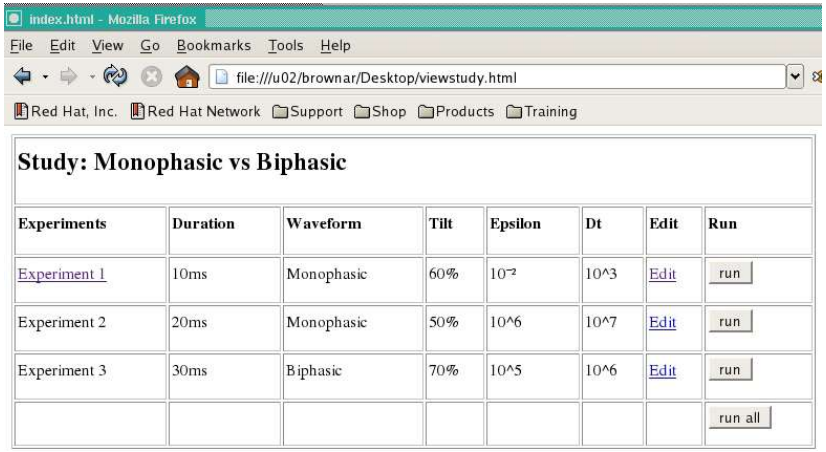


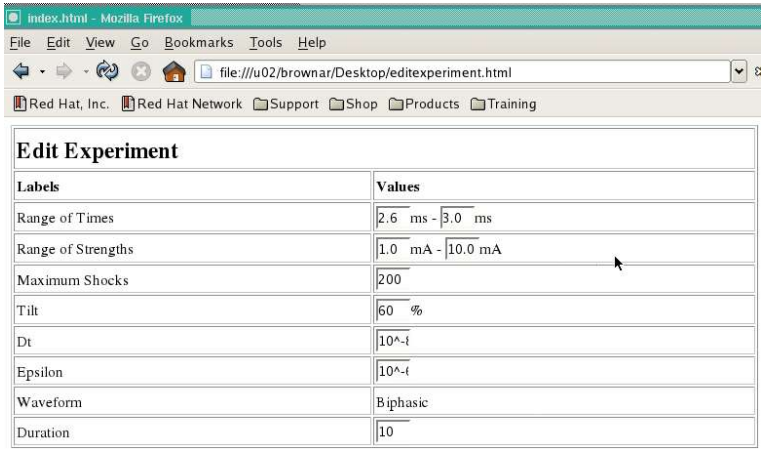
- Video observation of an individual scientific workflow at WLU
- Revealed the intricate nature of the process
- Helped identify what needs to be reproduced in the VRE

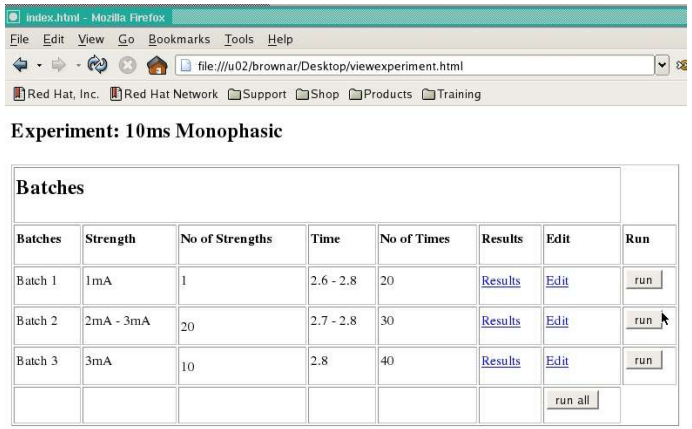
User interface design at WLU (1)

- 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.

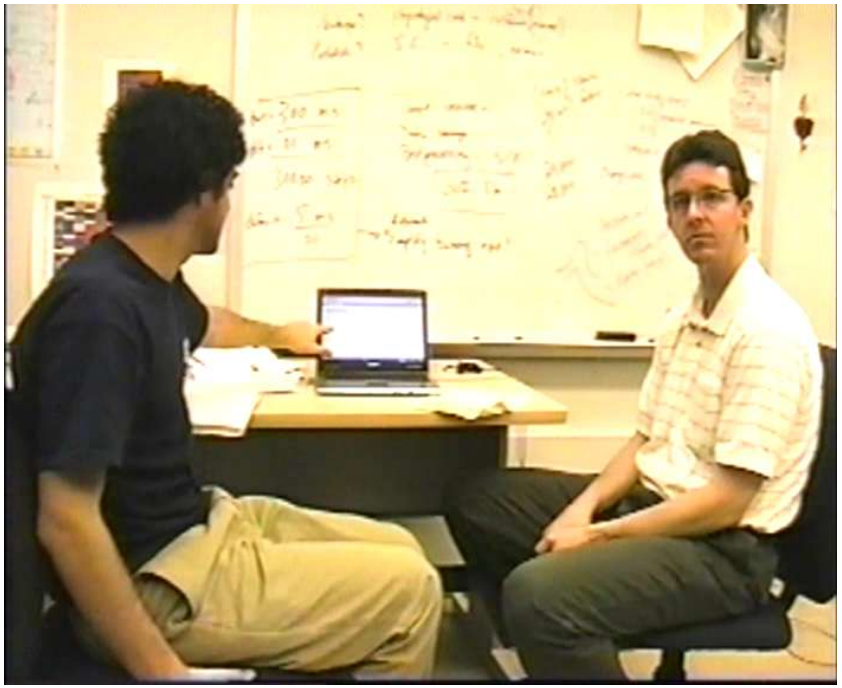
User interface design at WLU (3)





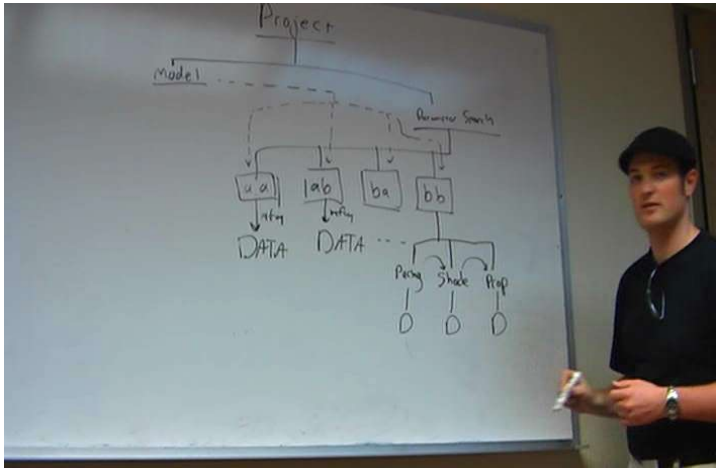


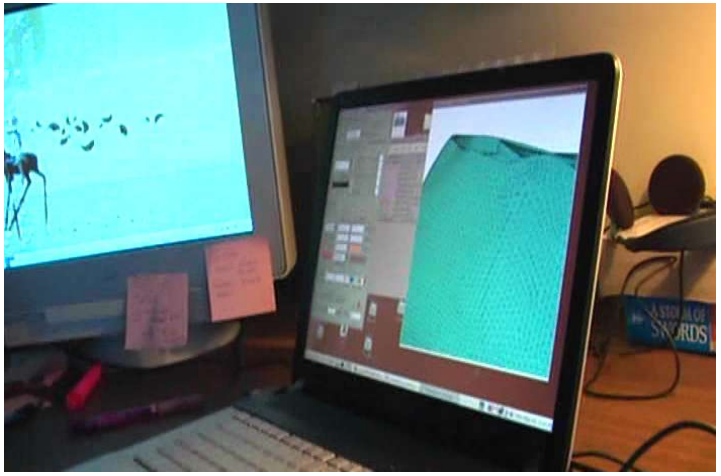
WLU UI Evaluation



- Evaluated with both an experienced and new student.

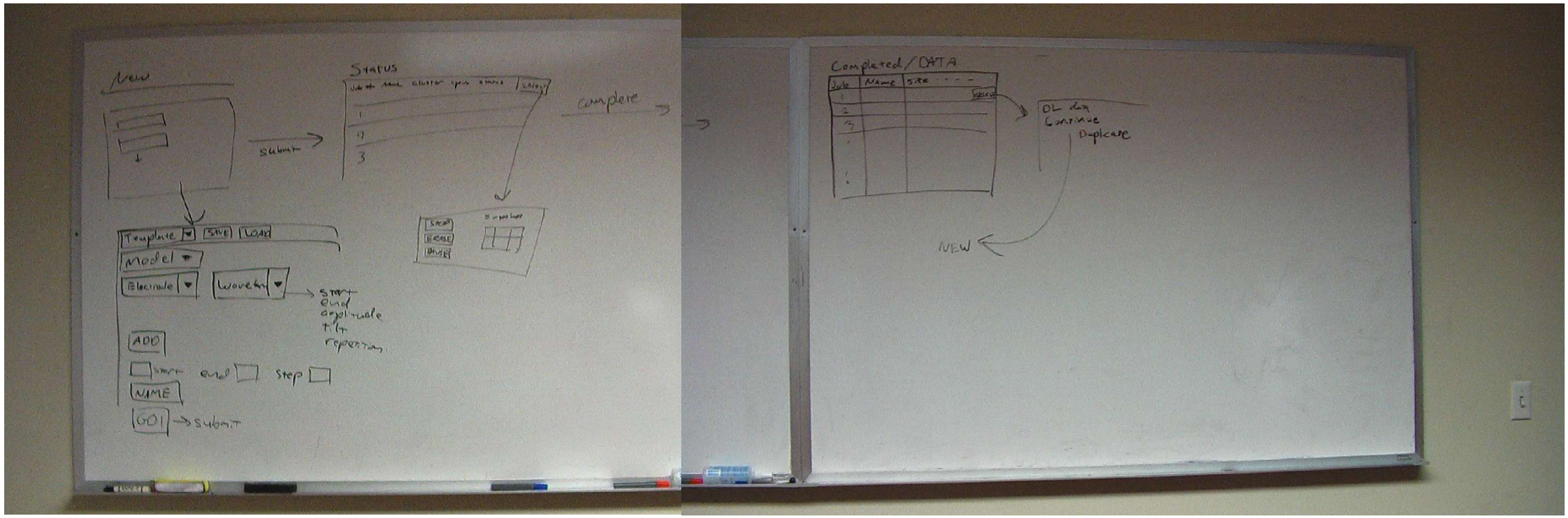
Design Workshop at Tulane University





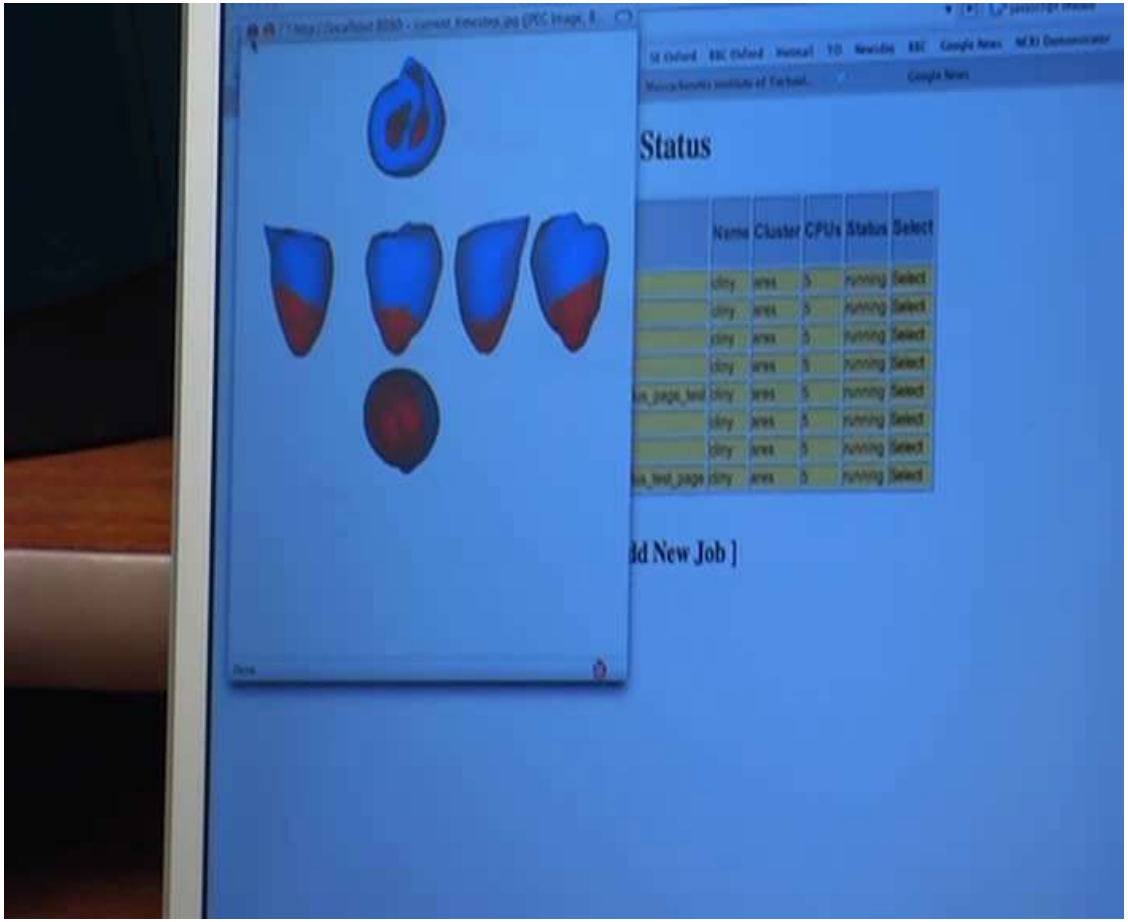
- Similar exercise at Tulane.
- Greater range of experiments.
- More generic solution required.
- Generic way to do parameter searches.

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.

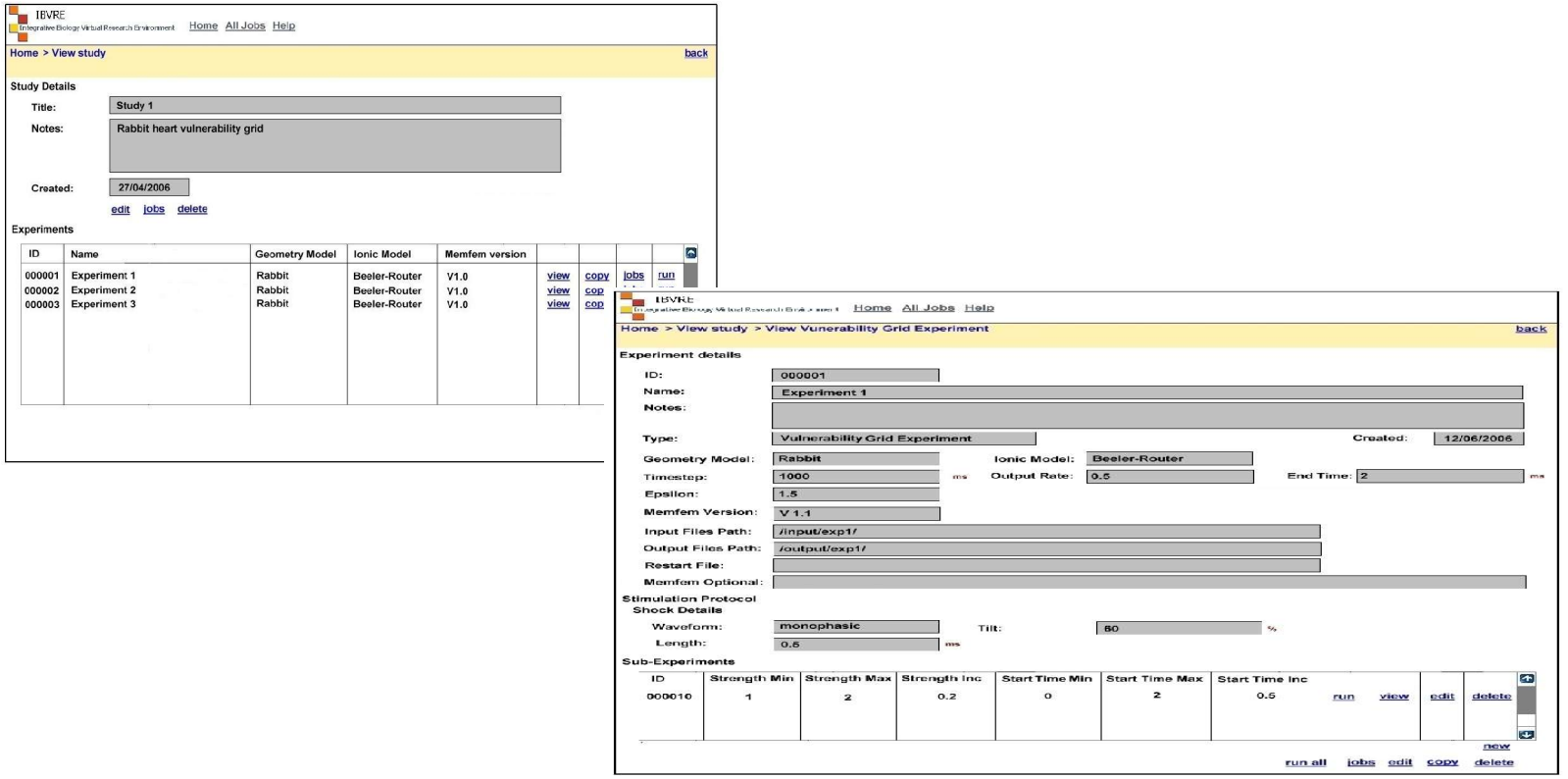
UI Design at Tulane (2)



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)



Digital Paper

- Logitech IO2 digital pens being evaluated with 11 heart and cancer modellers.
- Primary use-cases:
  - Heart: replacement for lab books.
  - Cancer: replacement for paper used for mathematical modelling.
- Benefits
  - Mathematical notes easier to retrieve
  - More amenable to sharing
  - Backup
- Preliminary data suggested other uses:
  - Using in conjunction with email
  - For use in supervisions
  - Drafting papers

Digital Paper - Evaluation

- Diary study.
- Interviews.
- Mini-workshop at the IB Project Workshop 2006
  - Participants in the evaluation
  - Invited other experts in this area
- Reporting back to
  - Academic community
  - Digital pen manufacturers

Finally... some other IBVRE Activities

- Collaborative visualisation: *Vannotea* – collaboration with Ronald Schroeter at the University of Queensland
- Paper notification tool – collaboration with Jasper Tredgold (ILRT, Bristol)

Thank You!

Project Website:

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

VRE Portal:

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