JISC

eResearch Australasia 2007

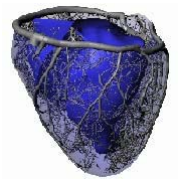
The JISC Integrative Biology VRE Project

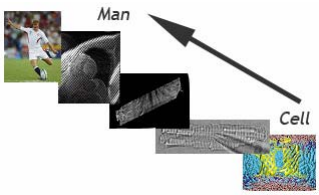
Dr. Ann Borda
JISC Programme Manager (e-Research)
a.borda@jisc.ac.uk

JISC

Overview - Integrative Biology (IB)

- IB is an EPSRC-funded e-Science project tackling UK's two biggest killers: cancer and cardiovascular 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.
- February 04 – January 08





JISC

Overview – Integrative Biology VRE (IBVRE)

- 2-year project funded by JISC (UK Joint Information Systems Committee), based at Oxford, started April 05 and ended March 07
- Developing a Virtual Research Environment (VRE) for the IB research consortium.
- To form a recognised visual gateway to underlying IB services (the IBVRE portal).
- Address user community needs not originally within the IB remit:
  - Supporting collaboration
  - Supporting the full research lifecycle

JISC

IBVRE Team

- Oxford University Computing Laboratory
- Oxford University Computing Services
- CCLRC (now STFC)
- Tulane University
- Washington and Lee University (WLU)
- Johns Hopkins University

JISC

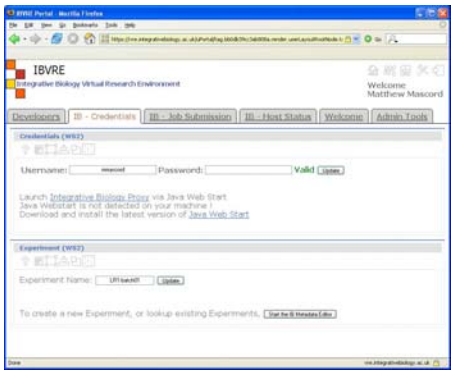
Initial work

- Two parallel strands:
  - IBVRE Infrastructure
    - Project management environment
    - VRE portal infrastructure
  - Research Process Analysis

JISC

Initial work – infrastructure development

- Migration of existing IB prototype portal (based on GridSphere) to a production quality uPortal installation
- uPortal chosen because:
  - Community movement and support
  - In-house (Oxford) experience
- Develop new look and feel.
- Hosting existing IB portlet tools.



JISC

Initial work – research process 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.

JISC

Initial work – research process analysis (2)

#	Requirement	Heart/Cancer	Method
1.	In Silico Experiment repository tool	Heart modellers	Bespoke development
2.	Paper material management tool	Heart & Cancer modellers	Evaluation of Anoto
3.	Visualization video collaborative analysis and annotation tool	Heart modellers	Vannotea Evaluation
4.	Literature alerting tool	Cancer modellers	Evaluation of SPP Literature Alerting tool

JISC

In silico experiment repository

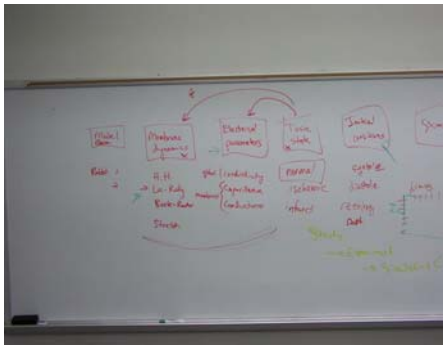
- To provide an interface allowing
  - Experiments to be designed and executed entirely through a visual interface without the need to use the command line.
  - The results from past experiments to be retrieved and easily reproduced.
- Meet specific needs first, to prove the concept, generalise later.
- 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)

JISC

- 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.

JISC

Research process storyboarding at WLU

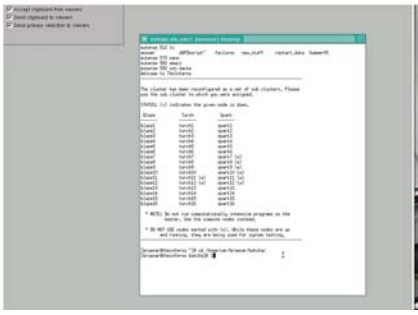


Divided experiment up into chunks.

Only a small number of parameters are modified across experiments.

JISC

Analysis of an individual's process at WLU



- Video observation of a 4th yr undergrad performing an *in silico* experiment at WLU
- Revealed the intricate nature of the process
- Helped identify what needs to be reproduced in the VRE

JISC

User interface design at WLU (1)

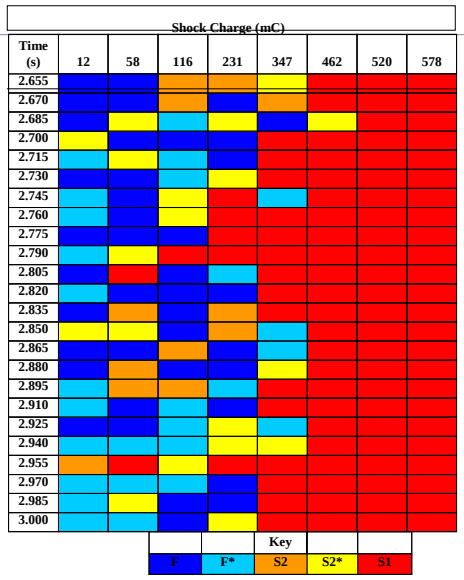
- Sketched out tailored interface for Vulnerability grid experiments
  - Experiments that test the affect of timing and strength of a shock applied to a simulated ventricle.

- Would work for a majority of simulations performed at the lab.

JISC

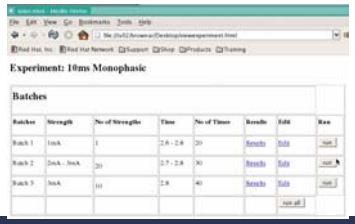
Why does the same strength shock sometimes succeed and other times fail to defibrillate?

- 200 simulations
- Each simulation independent of others
- 5000 CPU-hrs



JISC

User interface design at WLU (3)



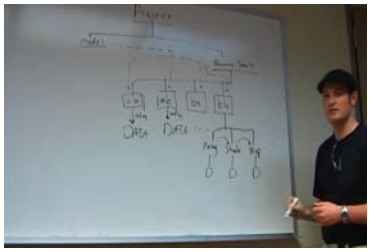
JISC

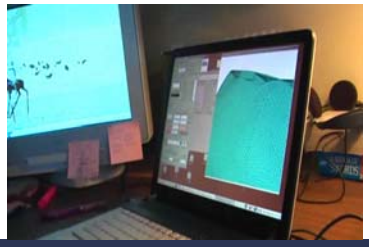
WLU UI Evaluation

- Evaluated with both an experienced and new student.

JISC

Design Workshop at Tulane University

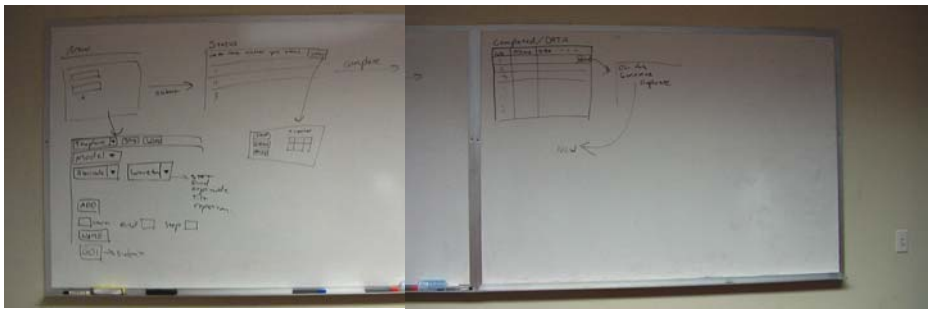




- Similar exercise at Tulane.
- Greater range of experiments.
- More generic solution required.
- Generic way to do parameter searches.

JISC

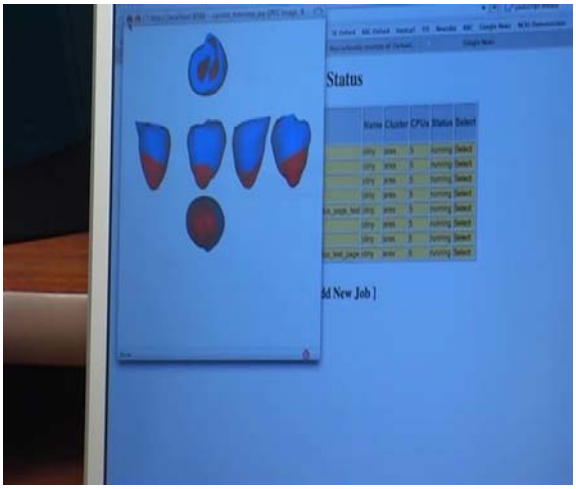
UI Design at Tulane (1)



- Result: off-screen visualisation rendering, exposed through the VRE.
- 6-way snapshot showing surface electrical activity.
- Generation of movies and stills from completed experiments.

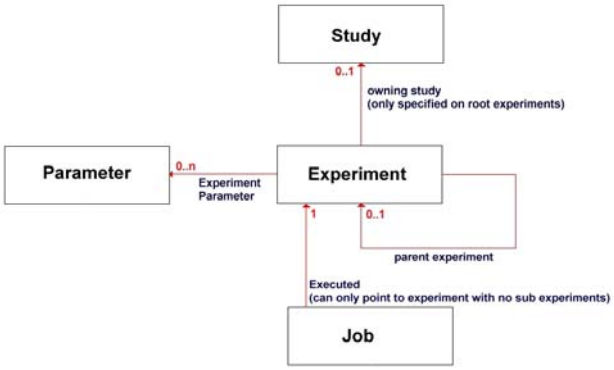
JISC

UI Design at Tulane (2)



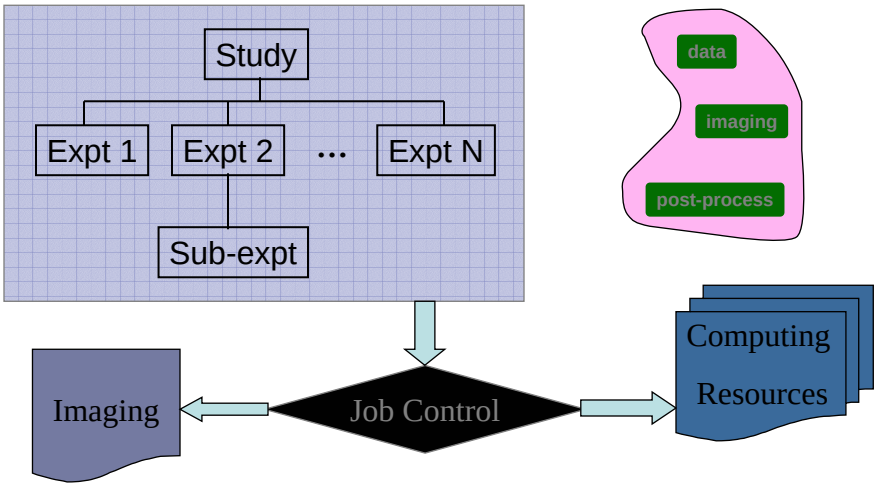
JISC

Subsequent development: IBVRE Data Model



JISC

IB Virtual Research Environment



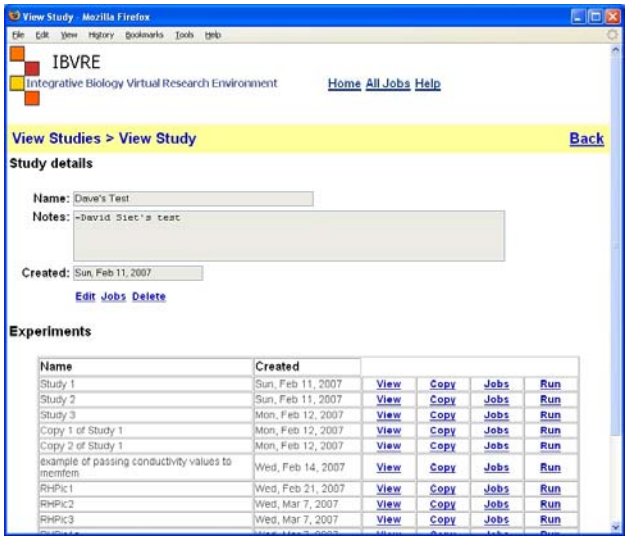
JISC

Subsequent Development (1)

- Design an interface bridging the requirements of the two groups.
- Link fully into IB web services infrastructure giving seamless access to SRB, NGS and HPCx.

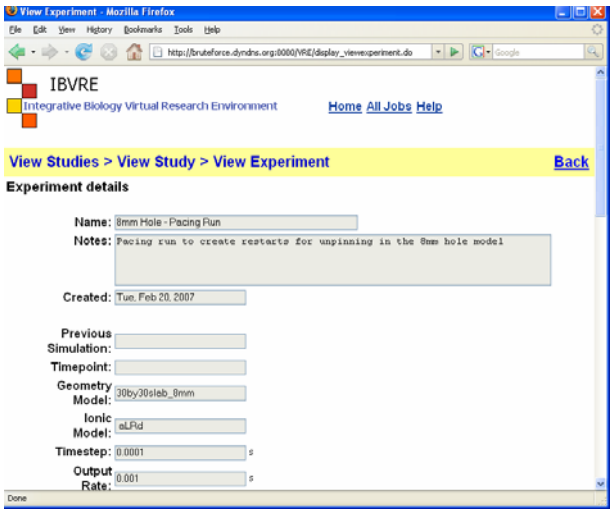
JISC

Subsequent Development - Interface



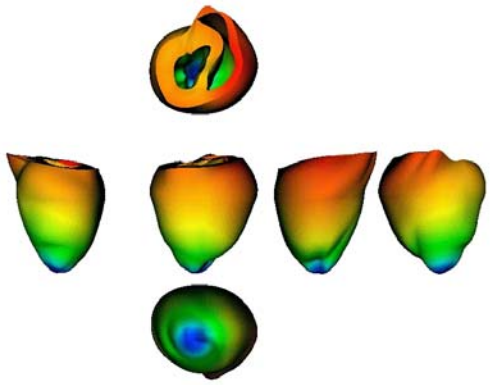
JISC

Subsequent Development - Interface



JISC

Subsequent Development – Snapshot feature



JISC

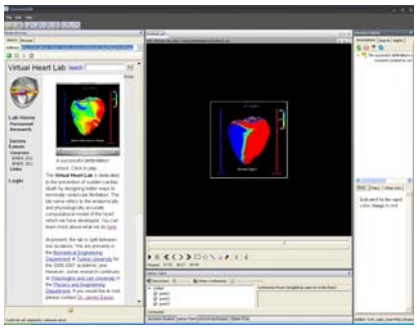
Key Features

- Ability to submit in silico simulation experiments without needing to use the command line.
- Automatic generation of input files, parameters and directories on the cluster.
- Visualization snapshot - implements a form of computational steering without needing to download data or use desktop visualization packages.
- Automatic creation and management of parameter-sweep style experiments, for example, Vulnerability Grid studies

JISC

Vannotea evaluation

- Collaborative visualisation: *Vannotea* – Oxford collaboration with Ronald Schroeter at the University of Queensland
  - Evaluation of tool using four heart videos for annotation and discussion



JISC

Conclusions

- VRE concept has great potential to transform work of integrative system biologists
  - simulation reproducibility and training of new researchers.
- In developing domain-specific VREs, identify and engage one or more 'customers' who have a good grasp of, and influence over, day-to-day research activities
- Collaborating with end user research groups by adopting the communication technologies and channels they themselves use
  - Wikis, IM, etc
- Involve end user research groups in the design and development phases, and in requirements analysis

JISC

Acknowledgements

With a special acknowledgement to Matthew Mascord

Project Manager of IBVRE

Project Website:

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

VRE Portal:

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

JISC

Contact Details

Matthew Mascord

IBVRE Project Manager

Matthew.Mascord@oucs.ox.ac.uk

Dr. Ann Borda

e-Research Programme Manager

A.Borda@jisc.ac.uk