

IBVRE

Integrative Biology Virtual Research Environment

JISC



The Integrative Biology VRE Project

User Requirements Gathering for the Humanities

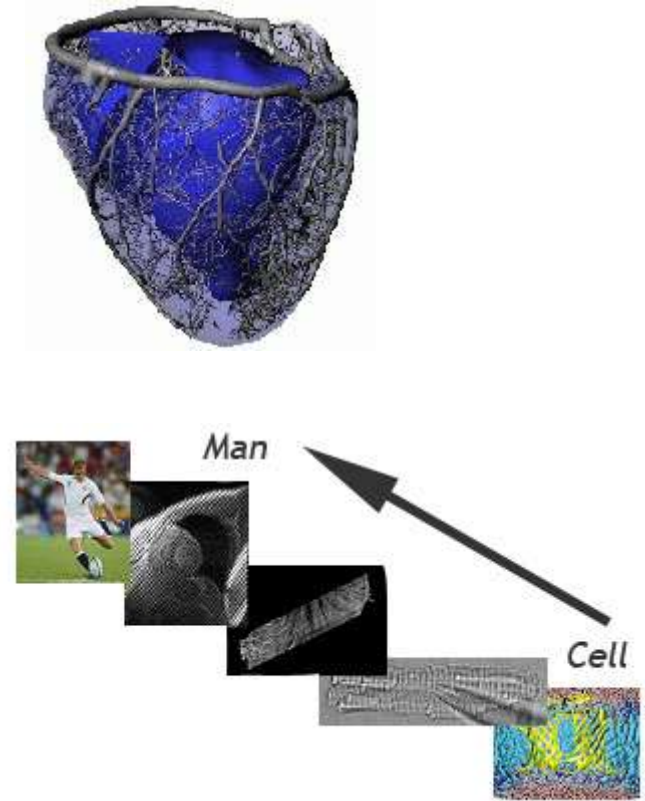
Workshop Two – Requirements Gathering in eScience

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 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

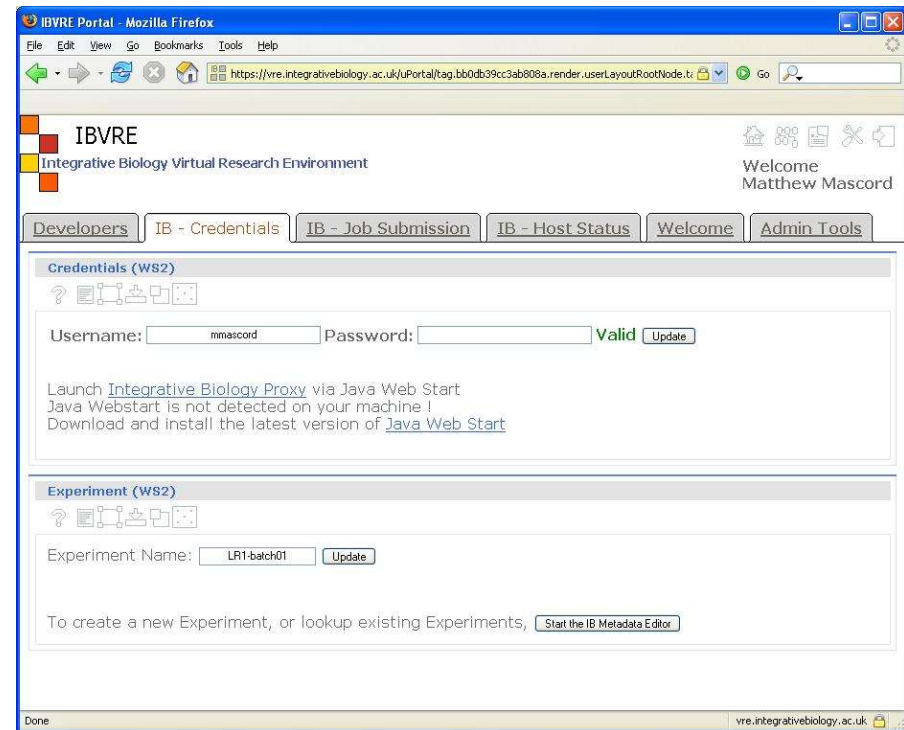
- PIs
 - Professor David Gavaghan, Project Director (Computing Laboratory)
 - Dr Andrew Simpson (Computing Laboratory)
 - Dr Michael Fraser (Computing Services)
- Core Staff
 - Matthew Mascord, Project Manager (Computing Services)
 - Geoff Williams, Developer – Systems (Computing Laboratory)
 - Clint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

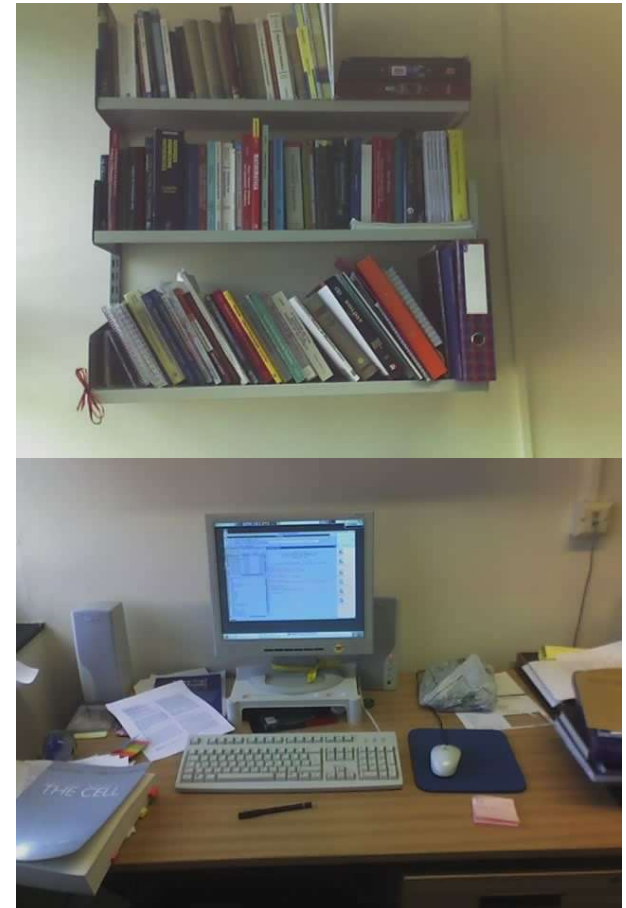
Initial work - development

- 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

```

 Accept clipboard from viewers
 Send clipboard to viewers
 Send primary selection to viewers

euterpe@wlu.edu:1 (browser) Desktop
euterpe 51% ls
answer: d@P@script failures new_stuff restart.data Sunner05
euterpe 51% nano
euterpe 55% emacs
euterpe 59% ssh dante
Welcome to TheInferno

The cluster has been reconfigured as a set of sub clusters. Please
use the sub cluster to which you were assigned.

STATUS: (x) indicates the given node is down.

Blaze      Torch      Spark
-----
blaze1     torch1     spark1
blaze2     torch2     spark2
blaze3     torch3     spark3
blaze4     torch4     spark4
blaze5     torch5     spark5
blaze6     torch6     spark6
blaze7     torch7     spark7 (u)
blaze8     torch8     spark8 (u)
blaze9     torch9     spark9 (u)
blaze10    torch10    spark10 (u)
blaze11    torch11 (u) spark11 (u)
blaze12    torch12 (u) spark12 (u)
blaze13    torch13    spark13
blaze14    torch14    spark14
blaze15    torch15    spark15
blaze16    torch16    spark16

* NOTE: Do not run computationally intensive programs on the
master. Use the compute nodes instead.

* DO NOT USE nodes marked with (u). While these nodes are up
and running, they are being used for system testing.

[browner@thesinferno ~]$ cd /home/var/browner/batchq/
[browner@thesinferno batchq]$ █
  
```



- 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)

index.html - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

file:///u02/brownar/Desktop/viewstudy.html

Red Hat, Inc. Red Hat Network Support Shop Products Training

Study: Monophasic vs Biphasic

Experiments	Duration	Waveform	Tilt	Epsilon	Dt	Edit	Run
Experiment 1	10ms	Monophasic	60%	10 ⁻²	10 ⁻³	Edit	<input type="button" value="run"/>
Experiment 2	20ms	Monophasic	50%	10 ⁻⁶	10 ⁻⁷	Edit	<input type="button" value="run"/>
Experiment 3	30ms	Biphasic	70%	10 ⁻⁵	10 ⁻⁶	Edit	<input type="button" value="run"/>
							<input type="button" value="run all"/>

index.html - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

file:///u02/brownar/Desktop/editexperiment.html

Red Hat, Inc. Red Hat Network Support Shop Products Training

Edit Experiment

Labels	Values
Range of Times	2.6 ms - 3.0 ms
Range of Strengths	1.0 mA - 10.0 mA
Maximum Shocks	200
Tilt	60 %
Dt	10 ⁻⁴
Epsilon	10 ⁻⁴
Waveform	Biphasic
Duration	10

index.html - Mozilla Firefox

File Edit View Go Bookmarks Tools Help

file:///u02/brownar/Desktop/viewexperiment.html

Red Hat, Inc. Red Hat Network Support Shop Products Training

Experiment: 10ms Monophasic

Batches

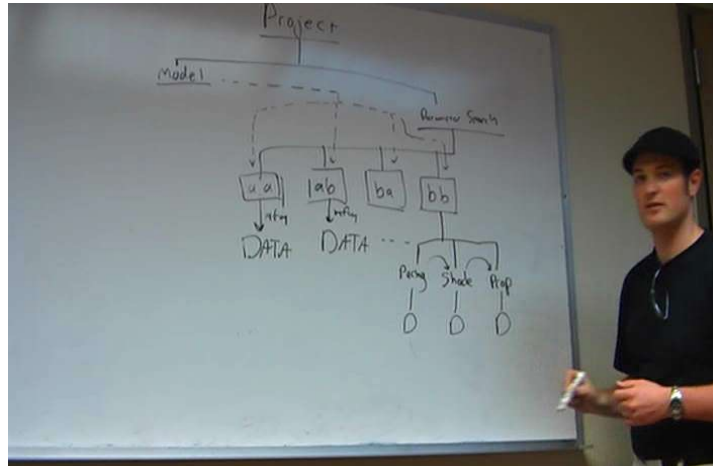
Batches	Strength	No of Strengths	Time	No of Times	Results	Edit	Run
Batch 1	1mA	1	2.6 - 2.8	20	Results	Edit	<input type="button" value="run"/>
Batch 2	2mA - 3mA	20	2.7 - 2.8	30	Results	Edit	<input type="button" value="run"/>
Batch 3	3mA	10	2.8	40	Results	Edit	<input type="button" value="run"/>
							<input type="button" value="run all"/>

WLU UI Evaluation

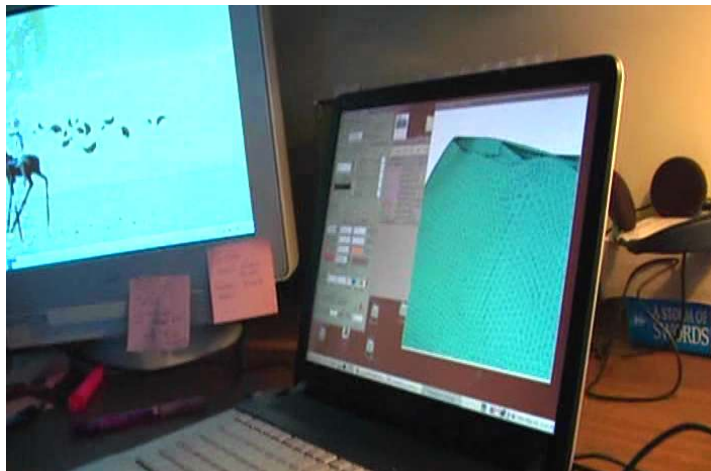


- Evaluated with both an experienced and new student.

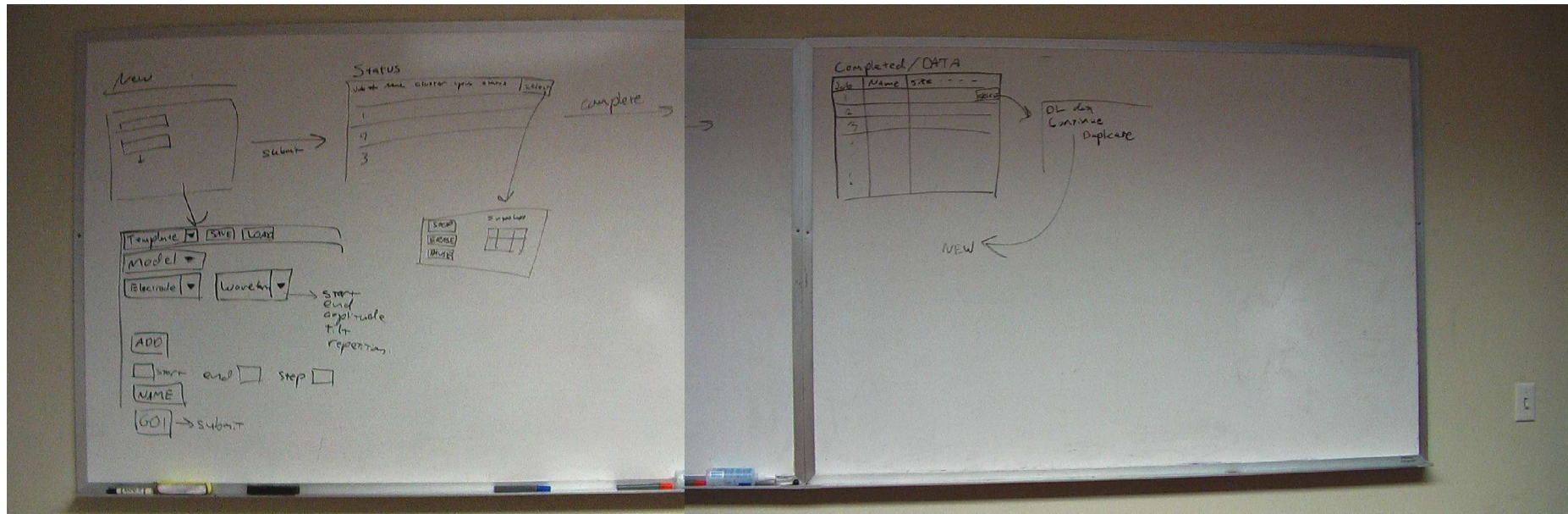
Design Workshop at Tulane University



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

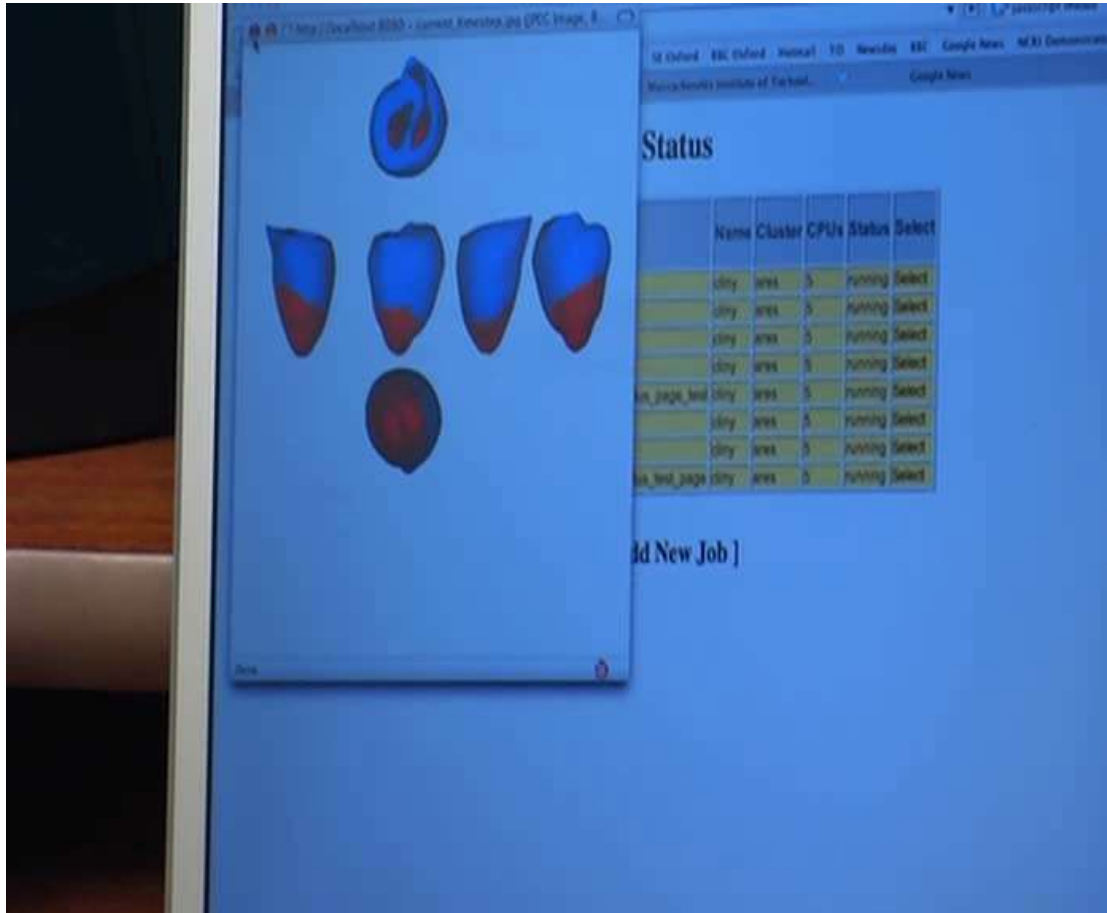


UI Design at Tulane (1)



- 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)

IBVRE
Integrative Biology Virtual Research Environment Home All Jobs Help

Home > View study [back](#)

Study Details

Title: Study 1

Notes: Rabbit heart vulnerability grid

Created: 27/04/2006

[edit](#) [jobs](#) [delete](#)

Experiments

ID	Name	Geometry Model	Ionic Model	Memfem version				
000001	Experiment 1	Rabbit	Beeler-Router	V1.0	view	copy	jobs	run
000002	Experiment 2	Rabbit	Beeler-Router	V1.0	view	copy		
000003	Experiment 3	Rabbit	Beeler-Router	V1.0	view	copy		

IBVRE
Integrative Biology Virtual Research Environment Home All Jobs Help

Home > View study > View Vulnerability Grid Experiment [back](#)

Experiment details

ID: 000001

Name: Experiment 1

Notes:

Type: Vulnerability Grid Experiment Created: 12/06/2006

Geometry Model: Rabbit Ionic Model: Beeler-Router

Timestop: 1000 ms Output Rate: 0.5 End Time: 2 ms

Epsilon: 1.5

Memfem Version: V 1.1

Input Files Path: /input/exp1/

Output Files Path: /output/exp1/

Restart File:

Memfem Optional:

Stimulation Protocol

Shock Details

Waveform: monophasic Tilt: 80 %

Length: 0.5 ms

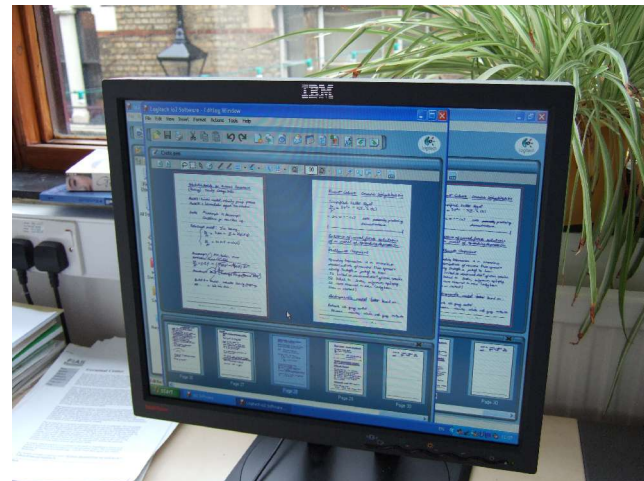
Sub-Experiments

ID	Strength Min	Strength Max	Strength Inc	Start Time Min	Start Time Max	Start Time Inc			
000010	1	2	0.2	0	2	0.5	run	view	edit delete

[run all](#) [jobs](#) [edit](#) [copy](#) [delete](#)

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/>