The JISC Integrative Biology VRE Project

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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 interdisciplinary community: US, Europe, New Zealand
- Developing a web-services based grid infrastructure providing tailored access to compute and data resources.
- February 04 – January 08
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

IBVRE Team

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

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

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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.
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.

Initial work – research process analysis (2)

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<th>Method</th>
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**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)

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**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.
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Research process storyboarding at WLU

Divided experiment up into chunks.
Only a small number of parameters are modified across experiments.

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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
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.

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

- 200 simulations
- Each simulation independent of others
- 5000 CPU-hrs
User interface design at WLU (3)

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

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

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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.
UI Design at Tulane (2)

Subsequent development: IBVRE Data Model
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.
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Subsequent Development – Snapshot feature

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
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

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
Acknowledgements

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

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

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