# JISC DEVELOPMENT PROGRAMMES

## Project Document Cover Sheet

## *IBVRE FINAL REPORT*

## Project

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## Document

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The project involved three departments at the University of Oxford: the Computing Services (through the Research Technologies Service), the Computing Laboratory, and the Oxford e-Science Centre (now the Oxford e-Research Centre). Towards the end of the project, the Council for the Central Laboratory of the Research Councils (CCLRC) joined as a project partner to assist in the completion of the Grid integration work.

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## Executive Summary

The Integrative Biology VRE project was a JISC funded Virtual Research Environment project based at the University of Oxford that ran for two years between April 2005 and March 2007. Led by Professor David Gavaghan, it aimed to investigate and develop the VRE concept in a computational biology setting by extending and complementing the work of the EPSRC Integrative Biology project.

The project's scope was initially open-ended but was then refined through a qualitative analysis of research processes across the IB community. This defined a programme of work based on bespoke technology development and third-party tool evaluation. The greater part of the work was the construction of a bespoke VRE interface and repository to manage the experimental processes of a distributed but closely collaborating group of heart modellers at Oxford, Tulane, Johns Hopkins and Washington and Lee University.

**Achievements**

1. The project has shown that the Virtual Research Environment concept is highly applicable to the integrative systems biology domain and that it can also be relevant in any discipline characterised by the need to run computationally intensive simulation experiments.

2. The VRE technology developed is already starting to have a major impact on the efficiency of biomedical research at three leading heart modelling groups around the world. By removing the need to develop complex scripts and manage compute resources, simulation experiments are more reproducible and easier to carry out by those lacking a high degree of technical expertise. In some cases, technical training time has been cut from up to a year to a matter of days, opening up this area of science to a wider community, including the teaching and learning communities.

3. Interest in the technology by the end user community has been demonstrated by the research groups' willingness to divert significant amounts of effort into ensuring the VRE worked correctly with their local compute resources as well developing the tool further to suit their individual needs.

4. The findings from the project's analysis of research processes have been of use, not only to this project, but also to several initiatives defining requirements at a broader level. Through the project's subsequent design elicitation workshops and evaluations, a comprehensive understanding of this community's ICT needs has been developed that is expected to be of great interest to future projects working in this area.

5. The project has actively disseminated its experiences and results at a variety of e-Research conferences and events, and through an article published in the Elsevier Future Generation Computing Systems journal.

**Conclusions**

1. The VRE concept has great potential to transform the work of those working in integrative system biology, particularly in the areas of simulation reproducibility and the training of new researchers.

2. When developing domain-specific VREs, it is crucial that one or more 'customers' who have a good grasp of, and influence over, day-to-day research activities, are identified and engaged, so the technology developed has a good chance of being taken up by the research community.

3. Involving end user research groups in the design and development phases as well as in requirements analysis can help develop a real sense of ownership over the end products, helping to encourage a wide adoption.

4. Collaborating with end user research groups can be facilitated by adopting the communication technologies and channels they themselves use to collaborate internally whether through the use of wikis, instant messaging, or internet phone.

5. The benefits of the current generation of portal technologies as a suitable presentation technology for VRE development have not been successfully proven by the work of this project.

# Background

The Integrative Biology VRE project was a JISC funded Virtual Research Environment project based at the University of Oxford that ran for two years between April 2005 and March 2007. Led by Professor David Gavaghan, it aimed to investigate and develop the VRE concept in a computational biology setting by extending and complementing the work of the EPSRC Integrative Biology project.

The Integrative Biology (IB) project is a second-round EPSRC e-Science Pilot project which commenced in February 2004 and is funded until January 2008. It received initial funding of £2.4M to support the research of nine post-doctoral researchers, and to provide training for 10 PhD students, across seven UK Institutions (the Universities of Oxford, Nottingham, Leeds, UCL, Birmingham and Sheffield, and CCLRC), IBM, and the University of Auckland. The IB project's scope is a combination of science and technology: on the science side, it aims to further understanding of the causes of cancer and cardiovascular disease through a combination of mathematical and computational modelling; on the technology side, it is building the underlying Grid infrastructure required to support this research. This infrastructure follows a service-oriented Grid architecture, and is utilising many of the middleware developments within the UK e-Science Programme and in the wider Grid community, and within the JISC Middleware programmes.

Whereas the IB project has focused on constructing a set of generic middleware services that can be composed to support a diverse range of activities, the Integrative Biology VRE project was set up specifically to investigate and address the user community's requirements in the areas of graphical user interfaces and collaborative tools, both pressing needs bearing in mind the distributed and collaborative nature of all of the research undertaken by this community.

# Aims and Objectives

The original aim of the IBVRE project was to investigate the utility of existing collaboration frameworks to support the entire research process of a large-scale, international research consortium - the EPSRC-funded Integrative Biology (IB) e-Science Pilot Project.

As elucidated in the original list of workpackages, the aim was not just to evaluate the chosen framework as-is, but also to acquire and develop tools that would then be plugged into this collaboration framework, supporting the scientific activities researchers in the IB community are actively engaged in.

These aims, in a broad sense have remained unchanged. Having said that, shifts in the technological landscape throughout the lifetime of the project have meant that, in some cases, the scope of some of the proposed activities has had to change.

### Choice of Collaboration Framework

In the IBVRE proposal, the Sakai Virtual Learning Environment [1] was named as the framework to use as a starting point. However, due to the number of other funded projects evaluating Sakai, it was suggested and subsequently agreed that IBVRE would evaluate OGCE 1.0 as an alternative.

OGCE 1.0 [2] is related to Sakai in the sense that both projects are derived from the same original code-base, namely the **C**ompre**H**ensive collaborativ**E F**ramework (CHEF) [3] from the University of Michigan[1]. The key value proposition of OGCE 1.0, in terms of its applicability as the basis of a VRE, is its core set of Grid-management and collaboration-facilitating tools. Crucially, as a result of OGCE 1.0 being built upon the Apache Jetspeed [4] portal framework, there was the facility to customise both the look and feel of the system, as well as the content and tools provided to the individual user.

Shortly after the IBVRE project commenced in April 2005, the development group behind OGCE 1.0 decided to change their strategy and discontinue the development and support of their collaboration framework, narrowing the scope of their activities in OGCE 2.0 to the development of a set of Grid

[1] Sakai is sometimes referred to as CHEF2.

management tools. We therefore had to identify an alternative collaboration framework to underlie the IBVRE, as it would clearly not make sense to adopt OGCE 1.0, an unsupported product.

uPortal [5] was a portal framework that at the time was being adopted by a range of other related projects, and was the framework used by three previous projects Oxford had been involved in: CREE [6], SPP[2] [7], and the internal OUCS Portal Project [8]. Moreover, the Sakai development team had recently decided to move towards a uPortal-based framework. This combination of factors led to the decision, agreed and approved by the JISC VRE Advisory Board, to adopt uPortal in preference to OGCE 1.0.

**Scope of Workpackages**

In the initial project plan submitted to JISC, the original workpackages were reworked slightly without changing the underlying content of the project. First, in order to make clearer the distinction between bespoke development carried out by the VRE development team itself and the integration and evaluation of tools produced by the IB technology group or other third parties, the 'Tool acquisition' workpackage was replaced with 'Bespoke tool development' to cover bespoke development only - any integration activities would be considered part of the 'Tool integration' workpackage.

Another change was the introduction of workpackage 6, the development of a tool management or process support layer, as a separate workpackage. The objective of workpackage 6 was to implement the interactions between the IBVRE tools to support the selected IB research processes. The final list of workpackages was as follows:

| # | Activity | Description |
|---|---|---|
| **1** | Project Management | Ongoing project management throughout the lifetime of the project. |
| **2** | IB research process selection and analysis | Identifying a list of prioritised requirements initially at a high level, and then moving down to a detailed level in the areas chosen for development, through design elicitation workshops. |
| **3** | IBVRE infrastructure development and maintenance | Developing and supporting the development infrastructure including the portal infrastructure. |
| **4** | Third party tool identification and integration. | Integrating third-party tools into the VRE to satisfy requirements emerging from workpackage 2. |
| **5** | Bespoke tool development | Bespoke development of tools to satisfy requirements emerging from workpackage 2. |
| **6** | Process support layer development and maintenance | Development of a tool management layer to support the requirements emerging from workpackage 2. |
| **7** | Evaluation | Evaluation of VRE middleware, bespoke and third-party tools, and project evaluation and reflection. |
| **8** | Dissemination | Ongoing dissemination throughout the lifetime of the project. |

Whereas workpackages 1, 2, 3, 7 and 8 were intended as ongoing activities throughout the lifetime of the project, the scope of workpackages 4-6 was deliberately kept open-ended, pending the completion of the workpackage 2, the initial phase of which was complete by November 2005.

At about the same time, some initial work was carried out in workpackage 4, to identify potential third-party tools that could be plugged into a VRE. As reported in the 2nd IBVRE progress report [9], this uncovered a severe shortage of relevant tools available in a portlet form. Subsequent work by the IBVRE systems developer revealed that, except in some limited scenarios, adapting non-portlet applications to run in portals can be both technically problematic and time-consuming. It was found that, in almost all cases, it is more efficient to completely re-write the user interface of the tool to be

[2]The SPP was originally built on Apache Jetspeed. A subsequent phase of the project investigated the reuse of SPP portlets within uPortal, an increasingly popular framework for supporting institutional portals.

natively portlet based. When considering that users had not expressed a strong desire for their existing tools to be integrated into a portal and the significant effort involved in doing this, it was decided that we must focus much more on bespoke development and evaluating third-party tools as-is rather than adapting them to work in a portal framework. The scope of workpackage 4 was consequently, much reduced.

Workpackage 2, the IB research process analysis activity, was a high level, qualitative analysis that benefited from a good level of participation from the IB community. It resulted in a project report [10] detailing 15 prioritised high level requirements and gave recommendations on how these requirements should be addressed. Once the initial analysis report was released in November 2005, a decision was made by the project board on the areas to address within the IBVRE project's timescale. A short-list was drawn up:

| # | Requirement | Target Community | Method |
|---|---|---|---|
| 1. | In Silico Experiment repository tool | Heart Modellers (Memfem Users Only) | Bespoke development |
| 2. | Paper material management tool | Heart & Cancer Modellers | Evaluation of Anoto Functionality |
| 3. | Visualization video collaborative analysis and annotation tool | Heart Modellers | Evaluation of Vannotea |
| 4. | Literature alerting tool | Cancer Modellers | Evaluation of SPP Literature Alerting Tool |

As this table illustrates, the planned work consisted of a combination of bespoke development combined with a series of smaller-scale evaluation activities. Addressing the in silico experiment repository requirement would cover the most part of workpackages 5 and 6, and considering the reduced scope of workpackage 4, the majority of work of the project. It is important to note that, to keep the scope manageable, the user community for the in silico experiment repository was restricted to users of Memfem, a nonlinear finite element simulation tool [11]. The evaluation of Anoto Functionality, the SPP literature alerting tool, Vannotea, and the in silico experiment repository would make up the majority of workpackage 7 - evaluation.

**Requirements Breakdown**

Further detail and background that led to the decision to build and evaluate these tools is given in the IBVRE Initial Analysis Report. However, the following overview outlines the need for each of these tools and their anticipated benefits.

Requirement #1: In Silico Experiment Repository

The anticipated benefits of the in silico experiment repository were to:

- Reduce the difficulties scientists have when reproducing the results from in silico experiments, typically derived from the need to interpret complex shell scripts - experiments are designed and executed almost entirely through a graphical web-based user interface;
- enable biologists to carry out simulations without needing a detailed understanding of cluster computing, Linux, or shell scripting, to reduce the ramp-up time for new researchers entering the field[3]; and
- open up this area of science to a wider audience, including the teaching and learning communities.

Requirements #2: Paper Material Management Tool

The need for the better management of paper-based material arose through consideration of some fundamental research practices in the IB community, particularly in the cancer modelling community. During our initial analysis of research processes, the use of pen and paper was identified as forming

[3] Before the VRE, a new researcher could typically spend up to a year gaining the necessary technical skills needed to run these experiments.

an essential component of research practice, either as the tool used to carry out the research - in the case of the IB mathematical biologists - or for the recording and managing of day to day research activities - in the case of the IB computational biologists. While the flexibility and convenience of paper may make it the most appropriate tool for capturing data in many situations, material captured on paper is hard to locate, search, and share with others. By evaluating Anoto functionality, a leading digital pen and paper technology based on the use of real paper and pen, we aimed to solve a range of very practical issues associated with the management of paper-based material, in addition to obtaining a more detailed understanding of these research practices and potential requirements for the integration of this technology within VREs.

Requirement #3: Visualization video collaborative analysis and annotation tool

Vannotea is a collaborative movie annotation and analysis tool developed originally as part of the FilmEd project, by the University of Queensland. The software allows multiple remote or co-present collaborators to synchronously play, discuss, and annotate movies. This functionality had been identified as particularly relevant to the IB project's heart modelers, who as a distributed group, frequently discuss videos of simulated and real heart tissue over the phone. This can often be problematic, as it is difficult for each person to start the movie at exactly the same time, and to know exactly which part of the movie is being discussed. As well as facilitating the discussion process, the other major benefit of the technology lies in its ability to record these sessions for the benefit of those not taking part in the discussion, and for future reference.

Requirement #4: Literature Alerting Tool

The need for a literature alerting tool emerged through a consideration of a major aspect of building and exploiting mathematical and computational models of biological systems - that of identifying data from the literature that can be plugged into these models as parameters. Data can literally come from any biology or medical-related journal, making it impossible to trawl through everything in order to find what you are looking for. Any tool that can alert the modeller to literature containing specific information has considerable potential to facilitate the modelling process.

## Methodology

The original approach for technical development involved three distinct activities:

(a) Collecting tools relevant to a particular research process
(b) Integrating them into the VRE
(c) Providing a tool management or process control layer.

Although the project aim moved much more towards bespoke tool development this overall methodology can be considered to have remained broadly the same. The in silico experiment repository is an implementation of the tool management layer, in the sense that it marshals underlying compute, data, and visualization services to achieve the same objective - supporting the research process. The only difference was that due to fundamental technical difficulties associated with integrating desktop applications into web applications, tools were not integrated into the VRE in a visual sense, only their underlying functionality. For example, one of the visualization packages used had a desktop user interface that could not be adapted for use within a portal or web application. We therefore worked with the developers of this tool to strip away the interface, leaving just the underlying rendering functionality, which we then integrated into the VRE.

### Technical Development Approach

In the early stages of the project, a number of different technical development approaches were researched in order to find a methodology most suitable for the project. This included a look at techniques from Extreme Programming [12] and Agile Software Development [13]. As one of the major risks to the project was always the potential lack of participation from the end user community, it was eventually decided that the project should follow a design methodology known as *Cooperative Design* [14], which is characterised by a high level of end user involvement. For this methodology to work, a high level of trust must be developed between developer and end-user, typically requiring frequent face to face contact.

The globally distributed nature of our user-base and cost of travel meant that we had to compress several short trips into intensive week-long design workshops at the end user labs. These workshops were planned to consist of a combination of research process analysis, observation work, collaborative user interface storyboarding and the iterative development and evaluation of throw-away UI mock-ups and prototypes. The intention was then to take away the detailed requirements elicited by evaluating these prototypes and together with the end-user groups, design, develop and evaluate a more generic solution.

**Choice of Presentation Technology**

The IBVRE project proposal stressed the use of portals, particularly those supporting JSR-168 [26] and WSRP [27], as the principal front-end technology of the VRE. However, it was also made clear that for some applications the limited functionality possible within portlets would not be sufficient for more in depth activities such as the construction of an in silico experiment, or the interactive visualization of complex data sets. Taking this into consideration our approach has evolved to develop the portal as a 'first port of call', designed to visually co-locate a set of resources relating to the user's day-to-day research activities. To support more complex activities, that would normally demand a full-screen view, more conventional web or desktop applications would be developed.

Problems encountered by the development team in obtaining a stable version of WSRP4J, the reference implementation of WSRP, combined with the lack of any practical requirement to use it, led to the decision to abandon WSRP in favour of developing straight JSR-168 compliant portlets. This led to a compromise of our original intended VRE architecture, which featured WSRP as the communication mechanism used between the portlet container and the portal.

**Evaluation Methodology**

A range of different approaches were adopted in evaluating the constituent IBVRE tools, from simple observation to diary studies and walkthroughs. In each case, a method was chosen to suit both the nature of the tool and the expertise or technical knowledge of the user. For example, with confident and experienced users, simple observation, usually with the person under observation describing the process, would be sufficient. For the less experienced, who were perhaps using a tool for the first time, a guided walk-through would be carried out. In these cases, questions the user might ask were helpful in highlighting areas of ambiguity or confusion in the user interface. With the Anoto digital paper, the aim was for a longer study and so a diary study approach was adopted. This study was supplemented through a workshop, follow up interviews, and an online survey.

As noted in the preceding section, formative evaluation of the in silico experiment repository was designed to be fully built in to the technical development approach. Final summative evaluation of the in silico experiment repository was carried out in February 2007 and is documented below.

## Implementation

Although the project started in April 2005, the first 3 months were allocated to preparatory arrangements and to recruiting the Project Manager based at Oxford University Computing Services and the two developers based at the Computing Laboratory. The core project team was therefore only fully complete in August 2005 - it comprised:

- Matthew Mascord, the project manager, based at the Oxford University Computing Services (started 1 July 2005).
- Geoff Williams, the systems developer, based at the Computing Laboratory (started 1 May 2005)
- Clint Sieunarine, the user interface developer, based at the Computing Laboratory (started 1 August 2005)

In July 2005, the project manager prepared the initial project plan and website, and started work building links with related projects in Oxford, and presenting a poster at the 2nd VRE programme meeting. The systems developer, between May 2005 and July 2005, investigated the open standards and software components expected to underpin the IBVRE infrastructure, including the portal

technologies JSR-168, WSRP, WSRP4J, OGCE and uPortal; grid technologies Globus, NGS, and HPCx; and security technologies Shibboleth and MyProxy.

In August 2005, the initial IB research process analysis and infrastructure development began in parallel, with the intention to have the development infrastructure complete as soon as high level requirements had been identified.

**Initial Research Process Analysis**

The initial research process analysis was organised between August and November 2005 and was carried out by the project manager in conjunction with the user interface developer. Dr Marina Jirotka from the Oxford Centre for Requirements and Foundations joined the project at this time to assist in defining an effective requirements gathering methodology. As the project proposal had kept its scope relatively open ended, not prescribing the development of any particular set of tools, we decided that a qualitative approach based on interviews and focus groups would be the most appropriate way to allow the analysis team to probe for more information where necessary.

The geographically distributed nature of the end user community, combined with their busy work schedules and budget constraints made it difficult to engage researchers across the IB community. Fortunately, the nature of their collaboration meant that non-UK researchers would often work very closely with colleagues based in Oxford, who could adequately represent their needs. For example, Peter Hunter's group in Auckland were represented through Chris Bradley who had been heavily involved in the development of CMISS - an electro-mechanical computational model of the heart. Natalia Trayanova's group at Tulane University were initially represented through Blanca Rodriguez who from the Computing Laboratory in Oxford, worked very closely with several members of the lab. Blanca had previously spent time working at Tulane as a post doctoral researcher.

The lack of contact with non-UK researchers was also partially redressed through the IB project workshop, held over two days in September 2005, which brought together in Oxford, a large proportion of the heart and cancer modelling research community. In cooperation with the IB project, we used this event as an opportunity to conduct a focus group to elicit and prioritise a set of high level requirements. Participating in this were representatives from Tulane (New Orleans), Graz (Austria), Nottingham, and W&L (Virginia).

**Initial Infrastructure and Portal Development**

Early infrastructure development carried out from July 2005 by the IBVRE systems developer included the installation of a Trac-based project management system and Subversion-based source code control system.

From August 2005, work moved towards taking over the support and development of the existing IB demonstrator portal, which was based on the GridSphere [15] portal framework and the NGS portal code-base, as a first approximation to a VRE. Technical work involved migration of the system onto a production quality uPortal installation, and the setting up of an automated test and integration environment at the Computing Laboratory in Oxford. Extensive system administration documentation was prepared by the systems developer and hosted on the project's internal wiki. The IBVRE user interface developer also assisted in this period by updating the look and feel of the existing system, re-branding it as the IBVRE. This updated system went live in January 2006.

Between December 2005 and February 2006, both before and after the installation of this new system, we carried out a series of evaluation exercises. The session before the installation was aimed at identifying any small-scale usability enhancements the IBVRE team could make, the sessions after were to evaluate the updated portal as a whole, to identify any issues users were having with these types of graphical user interfaces. These sessions were subsequently written up and made available on the IBVRE project website.

The main outcome from these evaluations was that, other than during the fairly artificial evaluation walkthroughs, users were resistant to using the portal in more realistic research situations. The reasons for this can be summarised as follows:

- The IB portal was a relatively thin layer over existing Grid services and did not provide sufficient additional benefits beyond what is available with the command line.
- Problems with 'Proxy Certificates', particularly creating and uploading them to the portal where they can be used to submit jobs to Grid resources on behalf of the user.
- Executing jobs through the portal was often more time consuming than through the command line.
- Being branded as a demonstrator, there was the perception that the service was not sufficiently robust for production use.
- Inertia - users will continue to use existing work practices despite shortcomings, due to the effort involved in changing them.
- Lack of understanding on how to use the portal - documentation.

We decided that in order to tackle these uptake problems, in addition to adopting the co-design methodologies eluded to earlier, the in silico experiment repository, which intended to replace many of the functions of the original IB portal, must be much more tailored to the individual research processes of our target user groups, and less generic.

As explained by Lee Momtahan in his report on VREs and Software Development [16], there are disadvantages to adopting this approach, but it was felt that following this approach, at least initially, would be the only way to secure a good level of participation, and get users to 'buy in' to the concept.

**Design Elicitation for the In Silico Repository Tool**

To keep the scope of this work manageable, the target user community for the in silico repository tool was restricted to those using the Memfem simulation software. Our pilot user community was chosen to comprise three of the largest labs around the world that use this tool on a day to day basis to conduct their simulation experiments:

- Computational Cardiac Electrophysiology Lab, Johns Hopkins University (Baltimore) (Professor Natalia Trayanova)
- Virtual Heart Lab, Washington and Lee University (Virginia) and Tulane University (Dr James C Eason)
- Computational Biology Group, Oxford University (Dr Blanca Rodriguez, Martin Bishop, Thushka Maharaj)

Natalia Trayanova's computational cardiac electrophysiology lab, the largest of the three labs, was originally based at Tulane University, New Orleans. Events in August 2005 led to them to relocate temporarily to the University of Washington at St Louis before returning to New Orleans in January 2006 and finally relocating permanently to Johns Hopkins University in August 2006. The Virtual Heart Lab, which was originally based at Washington and Lee University, relocated to Tulane University - with some work continuing at WLU - in July 2006 where Dr James Eason took up a visiting teaching position.

To these groups, this in silico experiment repository tool was marketed simply as the VRE - as we were not intending to provide any other tools. As such, the in silico experiment repository is referred to simply as the JHU VRE in the remainder of this document.

We had originally planned to conduct a single design elicitation workshop in January 2006, at Natalia Trayanova's lab, the largest of the three, inviting James Eason from Virginia along to participate. However, due to the lab's relocation to St Louis they were not in a position to accommodate us. Rather than wait, we decided to organise two separate workshops, the first at the Virtual Heart Lab in January 2006, the second at Natalia Trayanova's lab in May 2006.

At the January 2006 workshop, as planned, we carried out a combination of research process analysis, observation work, collaborative user interface storyboarding, rapid prototyping, and prototype evaluation. From February, the initial prototype was further developed from Oxford, with the team carrying out a series of shared desktop sessions with James Eason at WLU, to install and evaluate subsequent versions. The final outcome of this was that member of the lab there, Matt Kilansky, had managed to use the VRE successfully to submit a number of simulation studies to their

local computational cluster [17]. At the May workshop in Tulane, a similar approach was adopted, generating another proof-of-concept prototype tailored for the needs of this group.

Details of the outcomes of these workshops were written up and published on the IBVRE project website. In summary, the WLU lab required a tailored interface to allow the submission of so-called 'Vulnerability Grid' experiments. These are parameter sweep-style simulation experiments that test the combined effect of shock strength and timing when applied to a simulated heart ventricle. The Tulane lab wanted a much more generic interface to submit many different kinds of simulations. Their key need was the ability to produce a snapshot of the simulation, a visual representation of surface action potential, at the current time-step so decisions can be made on whether to continue or terminate the simulation, a form of computational steering [28].

Both the WLU and the Tulane prototypes were put together very rapidly and never designed to be robust - their main purpose was as a design elicitation tool. As such, subsequent work through June 2006 concentrated on taking these requirements and designing a more generic user interface alongside a data model to accommodate and bridge the needs of the two groups. This was carried out in conjunction with Rob Blake, the research analyst at the Tulane lab. Skype, IM, and digital pen and paper were used extensively in this period to help develop the design between Oxford and Tulane. The final design was then re-validated and refined with a number of Tulane lab members at a third mini-workshop held on 19 July 2006 at Tulane University as part of the IB Project world tour.

**Development of the JHU VRE**

By the end of July 2006, following the three design workshops, we felt we had obtained a reasonably detailed understanding of the requirements of the two groups and justified in committing to a longer period of development to allow time for a more robust infrastructure to be constructed. At this point, Rob Blake, who was heavily involved in IBVRE as part of the original September 2005 focus group, Tulane workshop, and in designing the user interface, left Tulane to take up a PhD course at the University of Illionois. In the subsequent development phases of the project from August 2006, we liaised with Umar Farooq who took over from Rob at Tulane.

Development work from August 2006 consisted of building a fully-functional web application based on the popular Apache Struts [18] web application framework, and a cut-down dashboard style version based on uPortal. The Technical Consultant (based in London) and the User Interface developer worked on the Struts version, while the Systems Developer worked on the portal version in parallel. Communication between project members normally took place through IM and email with Skype or phone used where more thorny issues arose. Where particularly difficult issues arose, morning design meetings were convened in Oxford. The technical design for the Struts application is based on the well known Model-View-Controller (MVC) [19] design pattern, with the data access layer (which provides the object-relational mapping) following the Core J2EE Data Access Object Pattern [29] and implemented using straight JDBC [20]. The portal version, by contrast, uses the Spring Framework [21] to implement MVC and Hibernate [22] to provide the object relational mapping.

In September 2006, the project was engaged in a number of dissemination activities, as detailed in the Dissemination section. At the IB project workshop, attended by Umar Farooq and Brock Tice from the JHU lab, we convened a meeting to discuss various technical matters relating to interfacing with the lab's computational cluster. In December 2006, a first version of the JHU VRE, which allowed submission of Memfem simulations to a single-node test cluster, was installed on a server at the Johns Hopkins lab. Umar Farooq assisted in this process by setting up the test environment - and also by continuing the development of the visualization snapshot functionality, originally developed in VTK [23] by Rob Blake. Again, in this phase, IM (AIM and Skype) were the main communication tools used throughout the deployment process.

At this point a few members of the lab started to try using the IBVRE to submit simulation experiments on a trial basis. Although some feedback had already been obtained through email, we felt it necessary to arrange a more formal evaluation to wrap up the project. A pre-evaluation session was initiated on 14 February 2007 as a three-way taped audio conference between Matthew Mascord (Oxford), James Eason (Tulane), and Brock Tice (Johns Hopkins). This, combined with follow up emails resolved some misconceptions users had had with the system leading to many giving up and losing interest.

The final formal evaluation was arranged as a video-taped shared desktop session utilising VNC and Skype on 16 February 2007. This was carried out between Matthew Mascord at Oxford and Brock Tice, James Eason, and David Siet - an undergraduate working with James Eason - at Tulane University. The session was organised around a guided walkthrough of the VRE, driven by David Siet, and subsequent general discussion. This session, combined with the earlier phone conference generated a coherent set of requirements for further development and was very reassuring in the sense that it validated the original VRE concept in its potential to transform the way the two labs work. It also spurred the two labs (particularly Brock, Umar, and James) into cooperating further to get the system working on their local production computational clusters.

**Managing Communication**

When not onsite, the different time-zones and researchers' busy work schedules meant that it could sometimes be difficult to keep up the momentum and a high level of user interest. One of the ways we attempted to overcome this was by using the communication channels lab members used themselves and were comfortable with. For example, at Tulane University, in Professor Natalia Trayanova's lab, a wiki was used on a day to day basis to manage all aspects of their research. In designing the VRE we chose to create pages within their wiki rather than using our own Trac wiki in the hope that this would be more successful in attracting input. This proved to be reasonably successful, although it meant that use of our original Trac wiki diminished except for documenting internal matters such as the system administration of project machines. All source code, however, was hosted on the IBVRE project management server in the Subversion repository, to which we gave several lab members access.

**Deployment Strategy**

Although it was initially envisaged that the JHU VRE pilot would be hosted in Oxford, after some thought, we took the decision to host the web application version at the end user institution with the aim to foster a greater sense of ownership over the end product. We also hoped that this would make it easier for the users to share the responsibility for maintaining and updating the application. The project team assisted the end user lab in this process by writing system administration and developer guides as pages within their wiki. This strategy was designed to contribute to the technology's sustainability beyond IBVRE in that the application would be supported through assistance not just from IB, but also by members of the end user research groups.

In contrast, the portal version of the JHU VRE was developed and hosted on the IBVRE test servers in Oxford.

**Integration of the JHU VRE with the IB Middleware Services**

In order to address the immediate requirements of our end user community, the first version of the JHU VRE was developed to work only with local computational clusters supporting the PBS queuing system. However, it was always planned that this prototype would be integrated with the middleware services developed by the IB Technology Group bringing the capability to submit simulation jobs to national Grid resources such as HPCx and the UK National Grid Service (NGS). These resources give additional computing power where local resources are unable to meet demand.

Integration of the JHU VRE with the IB middleware services, to provide this Grid connectivity, was originally planned to be carried out in conjunction with Damian Mac Randal, the IB Technical Architect and IB Technical Liaison on IBVRE. In October 2006 we received the sad news that Damian had passed away following a serious illness, having only recently been diagnosed.

By bringing on board CCLRC as a formal project partner between December 2006 and March 2007, we were able to fund Grid developers at the CCLRC e-Science Centre to complete his work. A version of the JHU VRE providing job submission capability to NGS, HPCx, and data hosting within the Storage Resource Broker (SRB) vault at CCLRC was installed on a server at Tulane University in March 2007, and was in alpha-testing at project end.

**Evaluation of Anoto Functionality**

The Anoto digital pen and paper evaluation was kick-started through a telephone conversation in January 2006 with Harry Yoshimura from Maxell Europe. Maxell kindly agreed to offer the project a Maxell DP-201 Pen Evaluation Kit free of charge, to be used for preliminary evaluation purposes. Between January 2006 and March 2006, we formulated a methodology for the main evaluation, and in April 2006 a preliminary diary study was conducted with two members of the Mathematical Institute at the University of Oxford.

Between July and September 2006 we gave twelve Logitech IO2 Digital Pens and a variety of Anoto paper products to members of the IB community at the Universities of Oxford and Nottingham. Evaluators were asked to use the back pages of their supplied digital notebooks to record their experiences with the technology through the course of the evaluation. These were reported back to the evaluation team through a mini-workshop on digital pen technology, follow-up interviews, and an online survey.

Full details on this evaluation and its findings were subsequently written up as, the IBVRE Digital Paper Evaluation Report in March 2007, available on the IBVRE project website.

**Evaluation of Vannotea**

We initially encountered difficulties identifying suitable candidates for the evaluation of Vannotea as few were using, or prepared to use Windows. Originally it was intended to conduct an evaluation involving participants in Oxford discussing movies with colleagues in the US. However, no one at the US labs used Windows, or even had access to it. We therefore had to identify suitable people in the UK with whom we could evaluate this technology.

Following an AccessGrid meeting in May 2006, Ronald Schroeter, the primary contact for Vannotea visited the Oxford on 11 July 2006. The current version was installed and demonstrated to Dr Blanca Rodriguez, a heart modeler based at the Oxford University Computing Laboratory; Blanca said she thought the tool had great potential in facilitating the discussions with her collaborators.

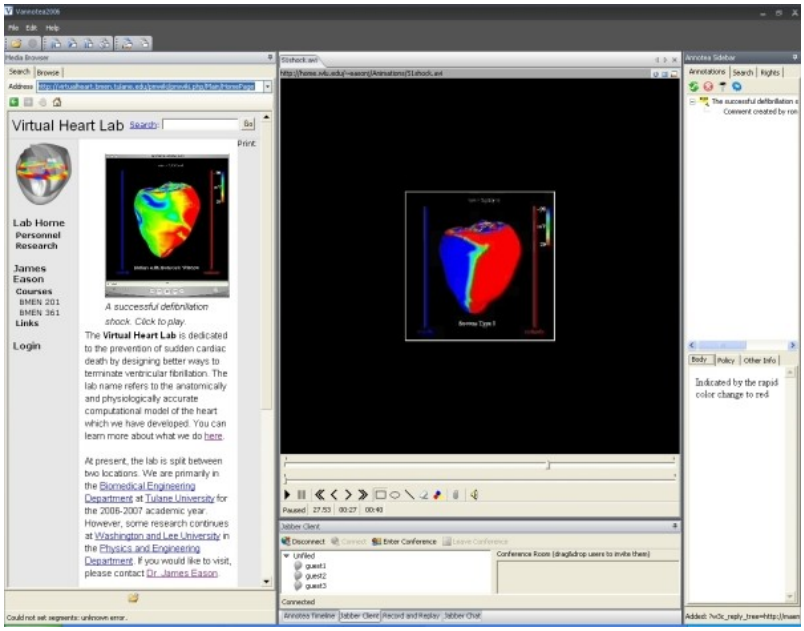

Figure 1 - Vannotea, showing a Heart Movie from the Virtual Heart Lab

On 28 March 2007, an evaluation was set up involving two members of the Computing Laboratory, and one member of the Department of Physiology, Anatomy and Genetics. Four heart videos of real scientific interest to them all were discussed over an audio link with Vannotea used to synchronise and annotate the videos between all the participants. An edited transcript of the discussion and issues and requirements it generated was subsequently written up and made available on the IBVRE project website.

### Evaluation of the SPP Literature Alerting Tool

The literature alerting tool was also originally planned as a bespoke development. However, we subsequently became aware of work by ILRT on the JISC-funded Subject Portals Project (SPP) that had tackled a similar problem. ILRT were planning to extend this work, from October 2006, to be more applicable to individual subject communities. After making contact with Jasper Tredgold at ILRT in July 2006, it was agreed that ILRT would work with the Integrative Biology VRE project to help define requirements, and once developed, the tool would be evaluated with interested users within the IB cancer modelling community.

In late December 2006, an initial set of screen designs were validated with a cancer modeller based at the Mathematical Institute and again in March 2006 where an initial prototype of the subscription user interface was made available (see Figure 2). Unfortunately, a version implementing email alerting was not available at project end and we were therefore unable to complete the evaluation of this tool as part of the IBVRE project.

Interest in the tool has nevertheless led to plans to continue this evaluation as part of the IB project with both the heart and cancer modellers, having emerged that the tool also has potential to benefit the heart modelling community even though they already have a number of existing large-scale models.

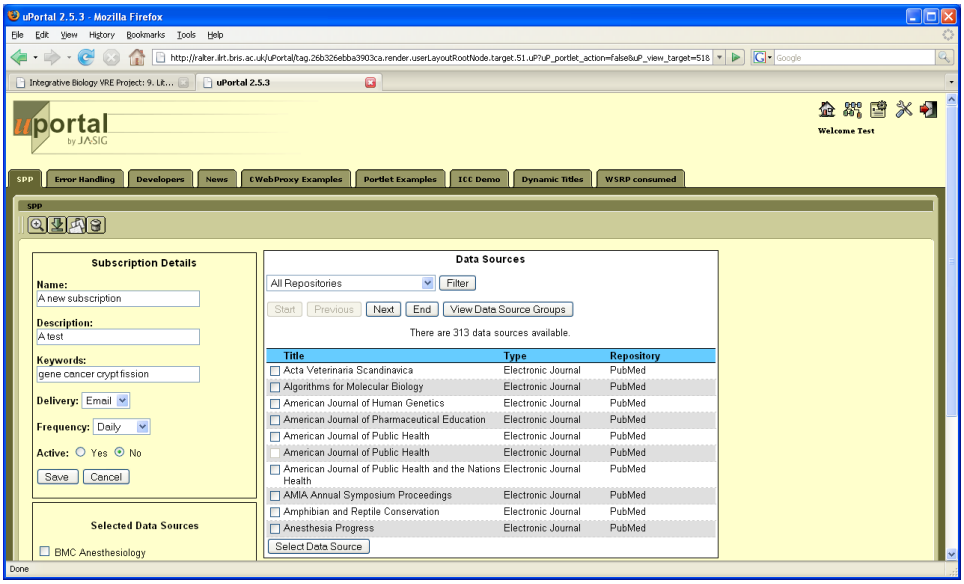

Figure 2 - the SPP Literature Alerting Tool, developed by ILRT

## Outputs and Results

The outputs of the project include both tangible software that is beginning to be actively used, combined with a set of evaluation reports on third-party tools, and VRE middleware technologies. The IBVRE project website (Figure 3) has acted as a place to record the project's status and disseminate its outputs as these have become available.

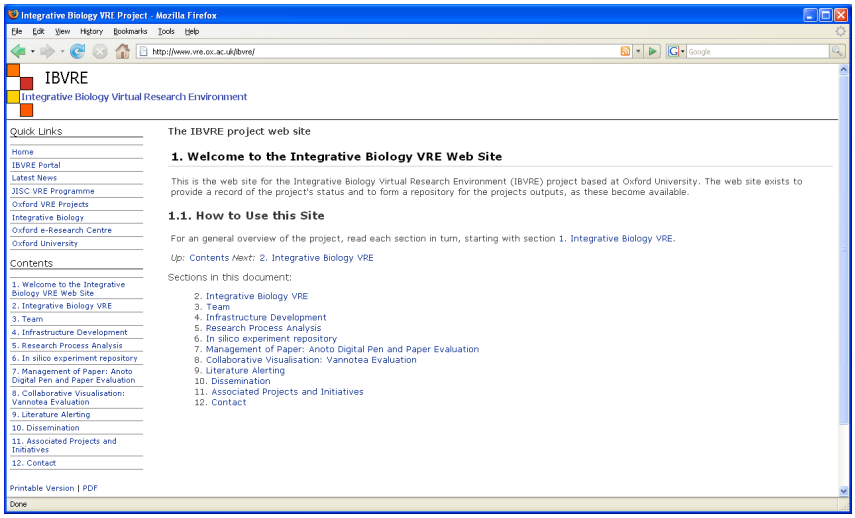

Figure 3 - IBVRE Project Website

**High Level Requirements**

The findings of the project's early analysis of research processes were published in November 2005 as the IBVRE Initial Analysis Report, available on the IBVRE project website.

The results from this study have been used both to define the scope of the IBVRE project but also to inform initiatives defining requirements at a broader level. For example, the University of Oxford used some of the findings of the study in the development of their ICT strategy [23], where they helped inform the development of a series of user scenarios.

The findings of the study also fed into the JISC-funded Intute Research Support Theme that aimed to ' undertake and publish an analysis of the needs of the research community with respect to online resource discovery in general and Intute in particular' [25].

**VRE at Johns Hopkins University (JHU VRE)**

This pilot system, hosted on a server at Johns Hopkins University, is now beginning to be actively used by a number of in silico experimentalists. Access is currently limited to current users of Memfem at Oxford, JHU and Tulane. Its key features are:

- 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 to show surface action potential at the current time-step of currently running simulations - without needing to download data or use desktop visualization packages.
- Automatic creation and management of parameter-sweep style experiments, for example, Vulnerability Grid studies.

Documentation relating to all three design workshops held at WLU and Tulane is available on the IBVRE project website.

The JHU VRE has a hierarchical structure where information is passed down the structure. The highest level is the Study. Under Study is Experiment and below that is Sub Experiment. Jobs (or simulations) can only be run from the lowest level. Variables defined at the Experiment level will be inherited by the Sub Experiment and cannot be changed. This data model is illustrated by Figure 4.

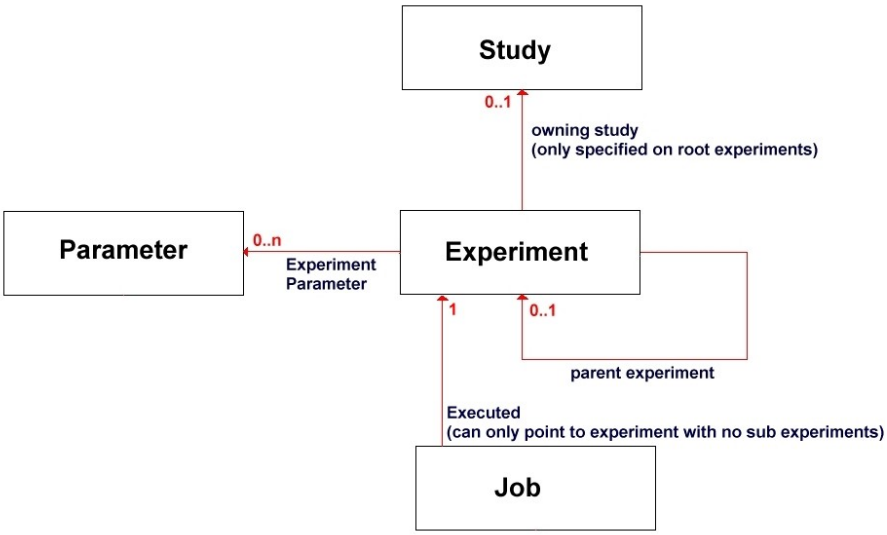


Figure 4 - IBVRE Data Model

The home page of the system, as shown in Figure 5, presents the user with a list of studies, each corresponding with a particular set of users. Each study has a view link, that takes the user to the View Study page, and a Jobs link that displays all jobs associated with the study. The All Jobs link at the top of the page displays all jobs associated with all the studies known to the system. The New Study link takes the user to a page allowing them to create a new study.

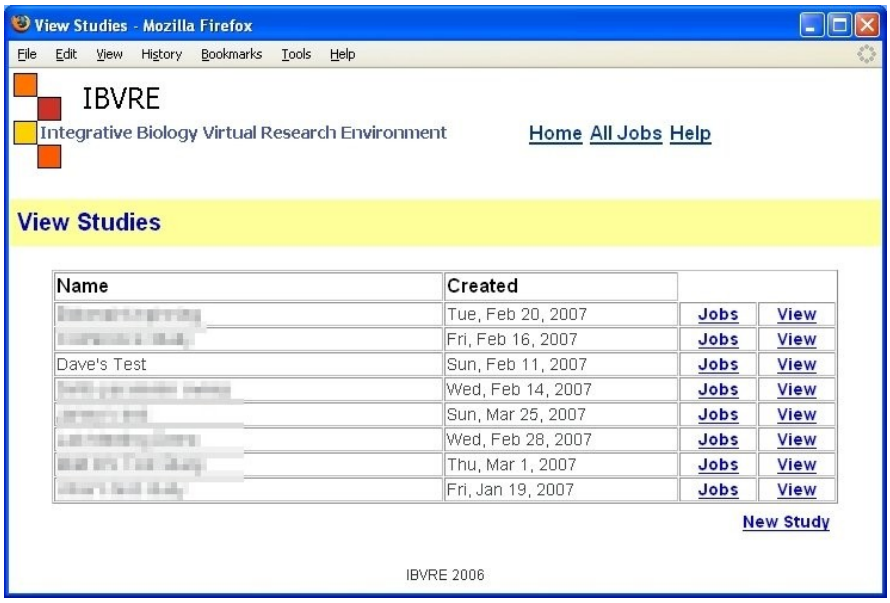


Figure 5 - IBVRE View Studies Page

The View Study page, as shown in Figure 6, displays descriptive information relating to the study and an edit link takes the user to a corresponding page allowing the user to edit this descriptive information. At the bottom of the page is a list of experiments associated with the study, each with a corresponding view link.

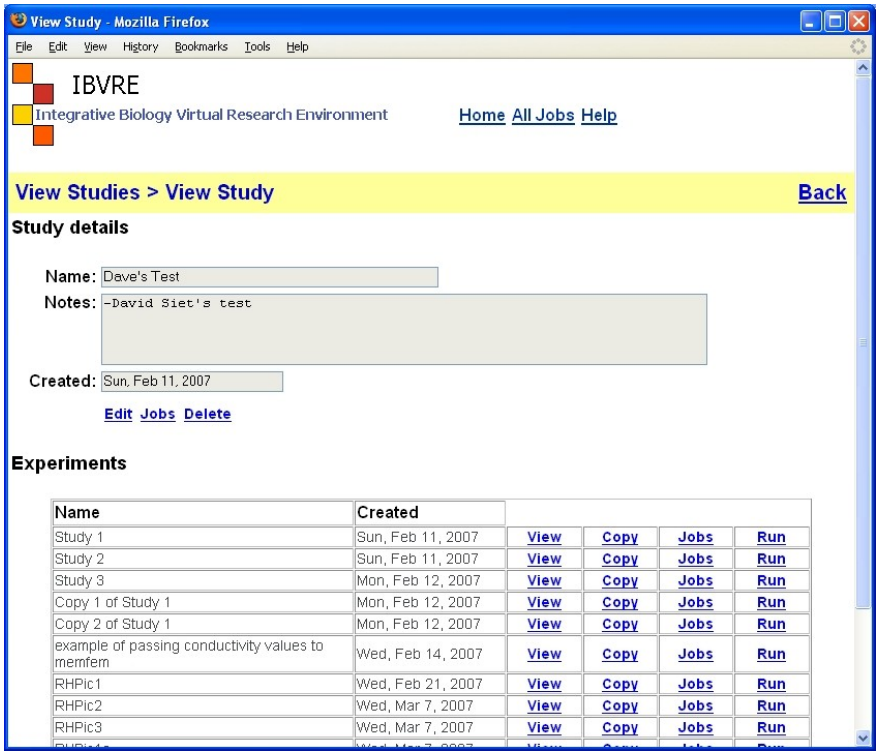

Figure 6 - IBVRE View Study Page

The View Experiment page, shown in Figure 7, lists the simulation parameters specific to the experiment, as well as a list of any immediate sub-experiments. A link at the bottom of this page, takes the user to another page, shown in Figure 8, listing all jobs associated with this experiment. An edit link takes the user to a corresponding page (not shown) enabling the user to edit the parameters associated with the experiment.

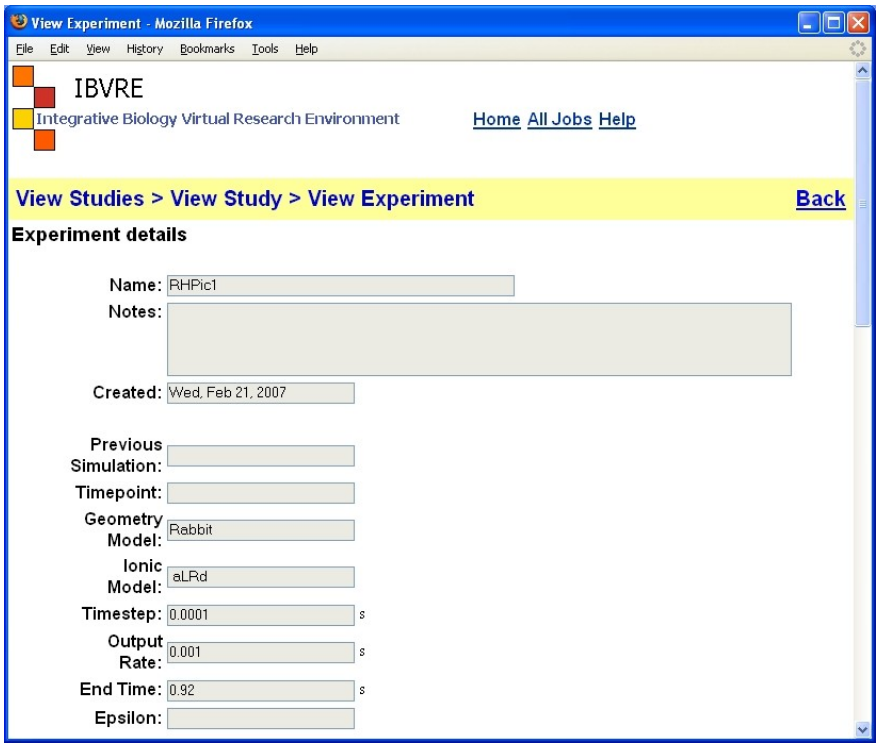

Figure 7 - IBVRE View Experiment Page


Figure 8 - IBVRE Experiment Jobs Page

Figure 9 shows the image returned when the user clicks on the snapshot link, one of the more innovative features of this VRE. This coloured image indicates the surface electro-potential at the current time-point of the running simulation, and helps the user to decide whether to continue with the current simulation or to abandon it.

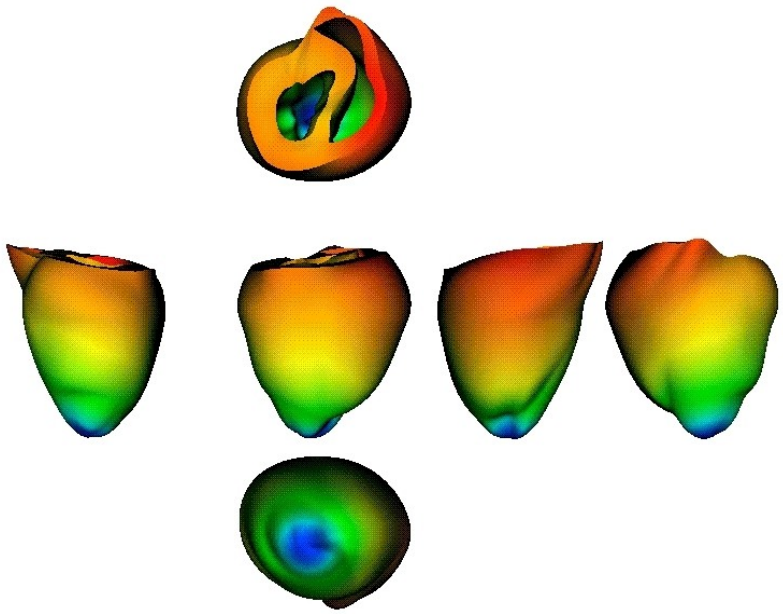

Figure 9 - IBVRE Visualization Snapshot

Current design, developer and user documentation is provided to the JHU lab via their wiki.

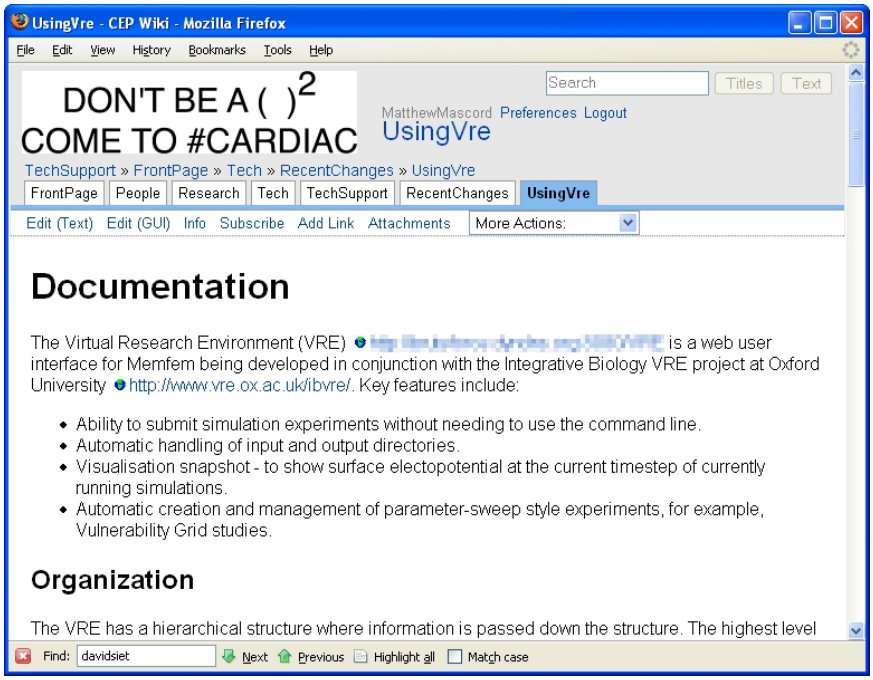

Figure 10 - User Documentation on the JHU wiki

A write up of the final formal evaluation of the JHU VRE, carried out in February 2007, is available on the IBVRE project website.

Source code for the system was released to the SourceForge [30] open source software hosting web site in March 2007, under the unix name ibvre. The software is being made available to the community under a Modified BSD licence (see Appendix B). Work will continue after project end to migrate the user documentation currently hosted on the JHU wiki to the SourceForge website.

The portlet version of the in silico experiment repository developed by the Systems Developer as part of an overall evaluation of portal technology, was still in development at project end and not ready for external release. Work will continue on this as part of the IB project, where there will be a focus on meeting the specific needs of the Computational Biology Group at the Oxford University Computing Laboratory.

A report on the integration of the VRE with the IB middleware services was being prepared by CCLRC at project end and will be made available on the IBVRE project website as soon as it has been completed, expected to be April 2007.

**Portal Technology**

The IBVRE JSR-168 compliant portal hosting the original generic IB Grid tools is available at <https://vre.integrativebiology.ac.uk>. Support for these tools has now been discontinued by the IB Technology Group, in light of their decision to focus on an FLTK desktop application providing similar functionality.

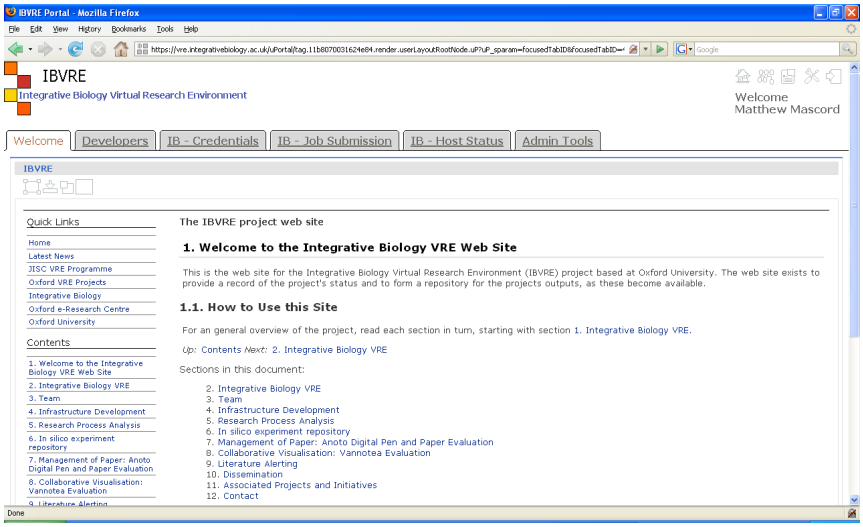

Figure 11 - IBVRE Portal

Documentation relating to the initial design of the IBVRE portal infrastructure, evaluation of the initial portal with the IB community, and a final evaluation of portal technology are available on the IBVRE project website in the following reports:

- IBVRE Initial Design Report, October 2005
- IBVRE Portal Evaluation Reports, December 2005 to February 2006
- IBVRE Portal Technology Evaluation Report, March 2007

### Evaluation of Third Party Tools

Reports on the evaluation of the third-party tools Anoto digital pen and paper, and Vannotea were published on the IBVRE project website in March and April 2007.

- IBVRE Vannotea Evaluation Report, March 2007
- IBVRE Digital Paper Evaluation Report, Matthew Mascord, Marina Jirotka, Annamaria Carusi, April 2007

### Project Reflection

A report on VREs and the wider software development process was commissioned by the IBVRE project as to serve as a reflection of the work of the project and how it may be sustained in future. The results of this are likely to be of interest to the wider VRE development community.

- VREs and Software Development, Lee Momtahan, March 2007

## Outcomes and Lessons Learned

The original aims and objectives of the IBVRE project were to build a virtual research environment that would look to support all aspects of the IB research lifecycle from identification of research idea all the way through to dissemination and provision of training. Following a consultation with the user community through workpackage 2, this scope was narrowed to support day to day activities rather than those that occur only once in a funding/research cycle. In the case of the heart modellers, this largely meant developing a bespoke VRE to support their *in silico* experimental process. For the cancer modellers it meant trialling Anoto digital pen and paper technology to assist in the management of their paper material generated through mathematical modelling.

### Time Spent Obtaining Requirements

The open-ended nature of the proposed project meant that a considerable amount of effort had to be devoted to requirements analysis - starting at a high level initially and moving down into a more

detailed analysis through the design workshops - before it was possible to start ramping up the development. It was not until December 2005, once the initial research process analysis was complete that a definitive set of tools had even been identified for development or evaluation. Subsequent delays completing the design workshops owing to Hurricane Katrina meant that the full and detailed set of requirements were only in place by the end of July 2006, leaving only six months to complete all development and evaluation work.

In hindsight, planning for a phased start-up may have been more efficient to enable developers to be brought in as and when needed. Though not planned for originally, this did occur to an extent in that the late start dates of project staff meant there was flexibility in the budget to bring in an experienced Java developer as Technical Consultant in June 2006 to assist in ramping up development. This flexibility proved critical to the success of the JHU VRE pilot.

**Impact of the JHU VRE Pilot on the Research Process**

The VRE is already starting to have an impact on the efficiency of biomedical research at Johns Hopkins and Tulane Universities. By removing the need to develop complex scripts and even use the command line, the process of constructing these *in silico* experiments has been greatly simplified, making experiments more reproducible, and making it far easier to train new researchers entering the field. Even at this early stage, members of the Tulane and Johns Hopkins labs are starting to use the system to conduct real science. Bearing in mind that the IBVRE team had, in reality, only six months to complete all the development and evaluation work - to get to this stage so early can be considered a significant achievement.

Further indicators of the success of the concept are attested to the fact that the JHU group has been willing to divert significant amounts of effort to extend and develop the tool further to suit their individual needs - something the VRE team has tried to encourage from the outset. The Tulane and JHU groups were so enthusiastic about the VRE concept that they even agreed to visit Oxford in March 2007 to actively 'sell' the technology to the IB community as part of an integrative biology project showcase event.

**Reflections on Working with Remote User Groups**

Working with user groups in the US, as expected, did present a number of challenges, not least in managing communication between the different time zones. Successful onsite design workshops at the two groups developed a high degree of trust between the users and the project team, but when the project team returned to Oxford between workshops or during a development phase, it would often be difficult to keep up the momentum and a high level of user interest. Often the success of the project can lie in keeping the interest of a small number of influential researchers and it can be very frustrating when these key people seem to lose interest.

For example, when we initially released a version in January 2007, although various users had tried to use the system, few had contacted us with feedback. It emerged later that this was because there had been some misunderstandings about some key features, which had led to these users giving up. When we arranged more formal evaluation sessions, involving walkthroughs, these misunderstandings came to light, and when the users had had another look at it in their own time, interest in the VRE concept was significantly renewed. This upturn in interest meant the group were prepared to get more involved in helping develop the solution, and were extremely cooperative when we attempted to get the system running on their production computational cluster.

Another set of difficulties the project faced was the transient nature of our user communities. The relocation of two of our end user labs in the middle of the project had a major impact on their attention towards the VRE work, as they were more concerned with the pressing need to set up their research infrastructure. However, on the positive side, the process of moving an entire lab meant lab members were already re-considering many of the ways in which they conducted their research. This, we believe, put them in the right frame of mind for thinking about how they might re-engineer their research processes in light of a VRE.

We found that in terms of the technology needed to support these evaluation sessions - Voice over IP (in this case Skype) and VNC combined with video recording proved invaluable. The lack of face to

face video contact was not seen as an issue as attention was mainly towards the tool under evaluation.

**An Understanding of the Generic Research Support Requirements**

Through developing and evaluating this VRE, the integrative systems biology community now has a much better understanding of its needs in terms of developing a generic collaborative user environment. At project outset, this was extremely hard to define beyond a basic need to manage data, computation, and visualization services.

We have complemented the bulk of the project work on this in silico experiment repository by evaluating a series of third party tools. These tools have addressed a number of other activities that occur throughout research, such as paper and proposal writing, and keeping laboratory notebooks. The effect of introducing these tools, as well as addressing a range of needs at a very practical level, has been to act as a probe into the domain that has led to a range of insights into the IB research process that would otherwise have been very hard to obtain.

Through our collaborations with related VRE projects (especially BVREH), we have identified areas of need that are common across a number of apparently unrelated subject disciplines. Identifying such common needs can help funding bodies such as JISC better prioritise their development agenda in the support of research.

## Dissemination

The project has conducted the following dissemination activities:

**Presentations, Posters, and Demos**

- Poster, 2nd VRE Programme Meeting, 6 July 2005
- A Virtual Research Environment for Integrative Biology: End-to-end Support for the Research Process, IB Workshop 2005, 30 September 2005
- Integrative Biology Virtual Research Environment, Research Technologies Service Tea Time Talk, 27 January 2006
- A Virtual Research Environment for the Integrative Biology Research Consortium (IBVRE), 3rd VRE Programme Meeting, University of Oxford, 16 January 2006
- Integrative Biology VRE, 4th VRE Programme Meeting, University of Manchester, 13 July 2006
- The Integrative Biology VRE Project: How portals and digital repositories can benefit computational biology, Digital Repositories, e-Research and Portals, Lancaster University, 6 September 2006
- The Place of the Digital Library within Virtual Research Environments, Digital Libraries a la Carte, International Ticer School (Tilburg), 24 August 2006
- Putting pen to paper: capturing the integrative biologist's paper trail, Poster, AHM2006, September 2006
- IBVRE Demo: JISC, EPSRC, and OeRC Booths, AHM2006, 19-21 September 2006.
- The Integrative Biology VRE Project, IB Workshop, 28 September 2006
- The Integrative Biology VRE Project, Repository Research and Implementation Workshop, Oxford University Computing Laboratory, 29 September 2006
- The Integrative Biology VRE Project, User Requirements Gathering for the Humanities, The Classics Centre, Oxford University, 12 October 2006
- The Integrative Biology VRE Project, OeRC Seminar, Berners-Lee Room, Oxford University Computing Services, 13 October 2006
- Piloting Virtual Research Environments at Oxford, Oxford University Library Services - Staff Conference 2007, St Catherine's College, Oxford, 15 March 2007
- A Virtual Research Environment for a Virtual Heart, Integrative Biology Showcase Event, Rutherford Appleton Laboratory, 27 March 2007

**Papers and Articles**

- Virtual Research Environments: Overview and Activity, Michael Fraser, Ariadne 44, July 2005

- VRE for the Integrative Biology Research Consortium (IBVRE), Portals Workshop, AHM2005, 19 September 2005
- Modelling the heart, Judy Redfearn, JISC Inform 14, July 2006
- Integrative Biology - the challenges of developing a collaborative research environment for heart and cancer modelling, Future Generation Computer Systems 23 457–465 (2007) doi:10.1016/j.future.2006.07.002

**Collaborations**

The IBVRE project's work has been of interest to a number of related projects internationally.

In September 2005, there was a visit from the Council of Australian University Directors of Information Technology (CAUDIT) where Oxford VRE work was presented. In October 2005, the project was visited by Dr Martie van Deventer, Knowledge, Learning & Information Officer at CSIR's Innovation Leadership & Learning Academy in Pretoria, South Africa. Dr van Deventer's interest was learning from the experiences of the project in an effort to establish the requirements for an eResearch support infrastructure for South African researchers.

In the course of the project we have collaborated closely with a number of related projects at Oxford and elsewhere. These included:

- Sakai VRE (Oxford)
- BVREH (Oxford)
- ELVI (Nottingham)
- SPP (ILRT, Bristol)
- ShibGrid (Oxford)
- Vannotea (University of Queensland)
- SUPER
- RIVER
- eReSS

## Conclusions

1. By carrying out bespoke development and third-party technology evaluation to address the highly particular needs of groups of closely collaborating heart and cancer modellers, we have shown that the VRE concept has great potential to transform the work of those working in integrative system biology, particularly in the areas of simulation reproducibility and the training of new researchers.

2. The key value proposition of JSR-168 and WSRP-based portal technology, that of providing a standard way to visually co-locate a set of disparate resources within a web browser, appears to be lost for domain-specific VREs, at least in this domain, where the user community is more interested in the provision of feature rich, tailored desktop or web applications that support the scientific tasks they are actively engaged in. In addition, the limited range of user interface interactions currently possible within JSR-168 portlets can seriously limit the usability of any interfaces developed. Use of portal technology by this community, we feel, is only likely to take off if the technology is adopted more widely by the IT industry as a whole and only after there is a critical mass of generally available portlet tools.

3. Experience on the IBVRE project has shown that identifying a 'customer' who can help steer and drive, at a detailed level, the course of the project is critical to ensure the project delivers something of real value to the community. In addition, it is crucial that those in the research community with a high level of influence over how research is conducted are engaged, so the technology developed has a good chance of being taken up.

4. When developing VRE solutions for a transient research community, adopting a cooperative design methodology (involving end users in the design and development process as well as in requirements analysis) to develop lightweight proof-of-concept prototypes as a design elicitation tool, and hosting the end products within the networks of the end-user institutions, can foster a

real sense of ownership by the end-user community over the solutions developed. This can help encourage a wide user take-up, as well as reducing the costs associated with maintaining and supporting a centrally managed service.

5. Collaborating with end user research groups can be facilitated by adopting the communication channels groups themselves use most to collaborate internally, for example, IM, wiki, or internet phone.

## Implications and Sustainability

1. There are a number of portals that have been designed to allow the submission of jobs to clusters, both to local resources, and to Grid resources. These portals tend to be fairly generic, and provide a relatively thin layer over the command line. In the IBVRE project we have built a more application-aware interface that operates at a higher level than managing the submission of individual jobs to compute resources, hiding much of these technical details from the end user

2. Making the IBVRE application aware has resulted in a high level of uptake in its target user community but at the cost of making it less immediately relevant to the wider community. However, as both the data model and the business logic layer of the system are simulation application agnostic with application-specific functionality encoded only at the level of the user interface, and encapsulated within special Executor java classes responsible for the translation of a set of generic parameter types into the command line arguments and input files required by the particular simulation executable, the system can be extended by others in future to support any discipline needing a more usable way to run computationally intensive simulation experiments.

3. The fact that we have made these technically demanding simulations easy to carry out, and reproduce has implications for the teaching and learning communities. Assuming simulation software writers agree to release their applications in source or binary form, such simulations can be encapsulated as learning objects to be used as a teaching aid for learners in any discipline characterised by a need to run computationally intensive simulations, for example, in biology, chemistry, earthquake engineering, materials science, etc.

4. In the immediate future, development of the IBVRE will be continuing both within the IB technology group until the end of the IB project in January 2008, and in individual user research groups. The IBVRE systems developer is continuing work on the portal version of the JHU VRE until the end of 2007 as part of the main IB project by focusing on developing a system tailored for the particular needs of the Computational Biology group at the Oxford University Computing Laboratory.

## Recommendations

1. The research, teaching and learning communities should push for the wider release of simulation software, in source or binary form, to encourage collaboration, increase the reproducibility of simulations, and to allow for the simulations to be encapsulated as learning objects for the benefit of the teaching and learning communities.

2. The research, teaching and learning communities should push for the developers of facilitating technologies to publish their file formats, to make it easier for the research communities to build tailored solutions where it is unprofitable for a commercial supplier to do so.

3. Future projects similar in scope to IBVRE should not attempt to write in and adopt too many immature or emerging standards and technologies. Flexibility should be introduced to allow relevant technologies to be selected only after a sufficiently detailed set of user requirements have been identified.

4. Future projects similar in scope to IBVRE may benefit from a phased start up to allow requirements and throw-away prototypes to be developed before development is ramped up.

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# Appendixes

### Appendix A - The IBVRE Consortium

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OUCL - Oxford University Computing Laboratory
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**Appendix B. IBVRE Source Code Licence - BSD**