

EPSRC e-Science Pilot Project in

Integrative Biology

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Overview of Talk

- Aims of the IB project
- Associated Projects
- Project Partners
- Graduate training
- Aims of the workshop

Key project goals

- To build an Integrative Biology Grid to support applications scientists addressing the key post-genomic aim of determining biological function
- To use this Grid to begin to tackle the two major research areas: the *in-silico* modelling of heart failure and of cancer.

The e-Science Challenge

- To build upon the first round of e-Science projects to build a virtual research environment to support the international integrative biology community
 - Goal is to provide the **grid infrastructure** to support scientists in providing seamless access to:
 - HPC resources (capacity and capability)
 - Computational steering
 - Data visualisation
 - Data management
- => Predictive *in-silico* models to guide experiment and, ultimately, design of novel drugs and treatment regimes

User Scenario

1. User (Ed) initiates in-silico experiment on HPC resource remotely from Canada using the VRE interface
2. IB system informs (electronically) collaborators in the US (Natalia and Jamie) and in Oxford (Peter and Blanca) that the experiment has commenced
3. Computational steering and visualisation libraries invoked to allow control of simulation as it progresses
4. Provenance and meta data concerning experiment is stored within IB databases
5. IB system monitors progress of simulation until some critical point is reached (e.g. initiation of arrhythmia) and notifies users
6. Ed initiates a collaborative steering session and all three members of the group can see the same visualisation of the progress of the simulation (Peter's is poorer quality)
7. A discussion via audio(visual) link ensues and several new jobs are spawned with parameter values covering a variety of possible treatment regimes (e.g. different functional forms of shock)
8. Steps 5-7 can be repeated or automated as required.
9. All simulations terminate. All simulation data, and associated metadata and provenance data, is automatically stored in the IB system for future analysis or post-processing.
10. The workflow describing the experiment is retained for future re-runs, editing, and use by "non-expert" users using MyIB tools.

Associated Projects/Proposals

- **MyGrid best practise**
- **ReG best practise**
- **VRE funding from JISC**
- **Sister Projects (EPSRC)**
- Adaptive FEM proposal
- SAN modelling proposal

Scientific Partners

- Heart Modelling
 - Auckland (Peter Hunter)
 - Calgary (Ed Vigmond)
 - UCLA (Alan Garfinkel)
 - UCSD (Andrew McCulloch)
 - Graz (Gernot Plank)
 - Oxford (Denis Noble, Peter Kohl, Blanca Rodriguez)
 - Sheffield (Richard Clayton)
 - Tulane (Natalia Trayanova, Rob Blake)
 - Utrecht (Sasha Panfilov, Kirsten ten Tusscher)
 - Washington and Lee (Jamie Eason)

Project Partners

- Cancer Modelling
 - Nottingham (Helen Byrne and colleagues)
 - Sheffield (Claire Lewis)
 - Oxford (Philip Maini, Jon Chapman, Chris Breward)
 - Birmingham (Marta Kwiatkowska, Eamonn Gaffney)
- Molecular Dynamics
 - Sansom Group in Oxford

Project Participants

- Project management
 - Sharon Lloyd (Oxford)
 - Damian Mac Randall (CCLRC)
 - David Boyd (Oxford)
 - David Gavaghan (Oxford)
 - Andrew Simpson (Oxford)
 - Lakshmi Sastry (CCLRC)

Project Participants

- Visualisation/Interactive Services/Grid services/Workflow
 - Lakshmi Sastry (CCLRC)
 - Sri Nagella
 - Ron Fowler
 - Ken Brodlie (Leeds)
 - James Handley
 - Peter Coveney (UCL)
 - Gianni di Fabritiis
 - Carole Goble (Manchester)

Project participants

- Software Engineering/Scientific/Parallel Computing and Numerical Analysis (Oxford)
 - Jon Whiteley
 - Joe Pitt-Francis
 - Alan Garny
 - Lee Momtahan
 - Jonathan Cooper
 - Thushka Maharaj
 - James Southern
 - James Osborne
 - Prasanna Pathmanathan
 - Chris Bradley
 - David Gavaghan

Project Participants

- Data management
 - Kirstin Kleese van Dam (CCLRC)
 - Daniel Hanlon (CCLRC)
- VRE Development
 - Matthew Mascord (Oxford)
 - Geoff Williams (Oxford)
 - Clint Sieunarine (Oxford)
 - Matthew Dovey (Oxford)
 - Rob Allan (CCLRC)
- Security
 - Andrew Martin (Oxford)

Graduate Training

- 9 PhD students have now joined the project having completed their training in the Oxford Doctoral Training Centre
 - Alex Fletcher (Oxford)
 - Alex Walter (Nottingham)
 - Chze Ling Wee (Oxford)
 - Ellie Boston (Birmingham)
 - Gary Mirams (Nottingham)
 - James Osborne (Oxford)
 - Jonathan Cooper (Oxford)
 - Nicolas Jeannequin (Oxford)
 - Philip Murray (Oxford)

Aims of this Workshop

- Thursday
 - Overview of the science

- Friday
 - Brief overview of the technical developments
 - Demonstrations and hands-on experience/tuition
 - Opportunity to feed back to the developers