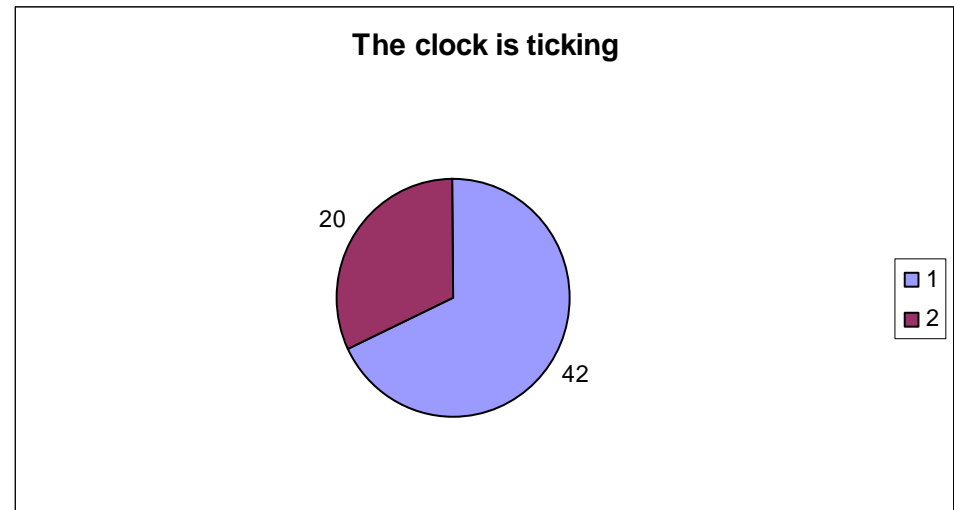


# Integrative Biology

## *Overview of Progress*

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Computing Laboratory  
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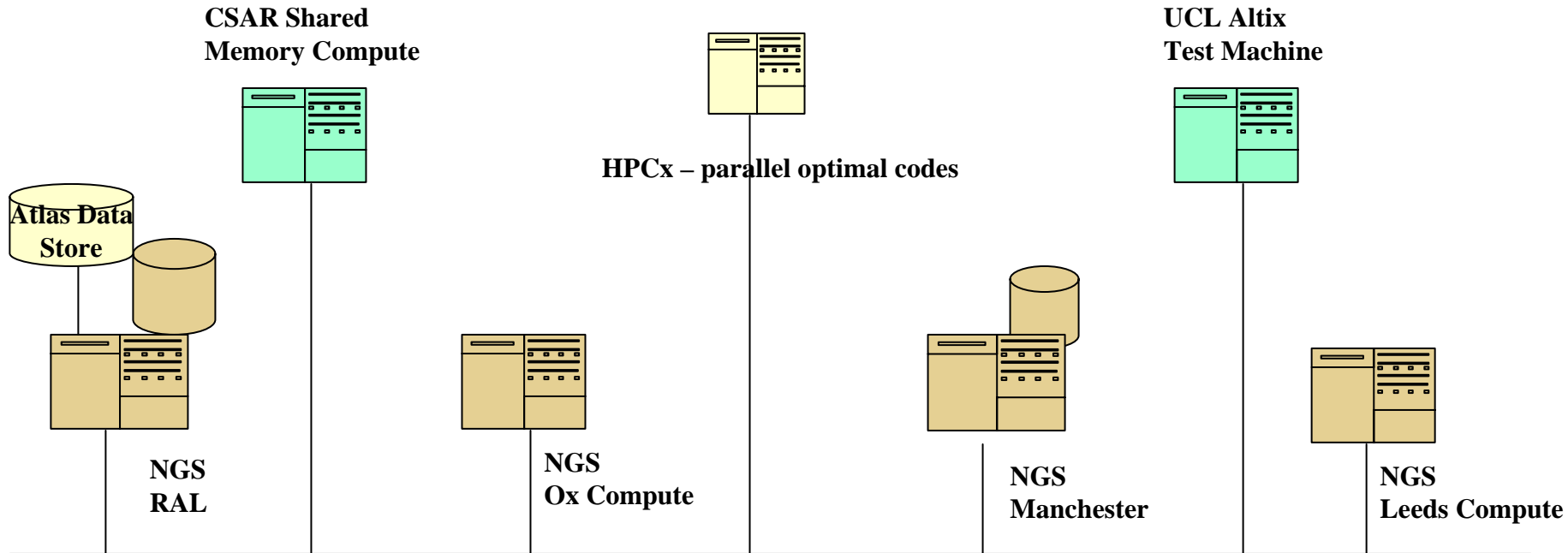
# Status Update

- Recap Objectives
- Approach
- Evolving Projects
- Successes with national compute resources
- Evolving Technology Team
- Demonstrating Here
- Plans 2005/6

## Recap Objectives

- 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 chosen Grand Challenge problems: the *in-silico* modelling of heart failure and of cancer.

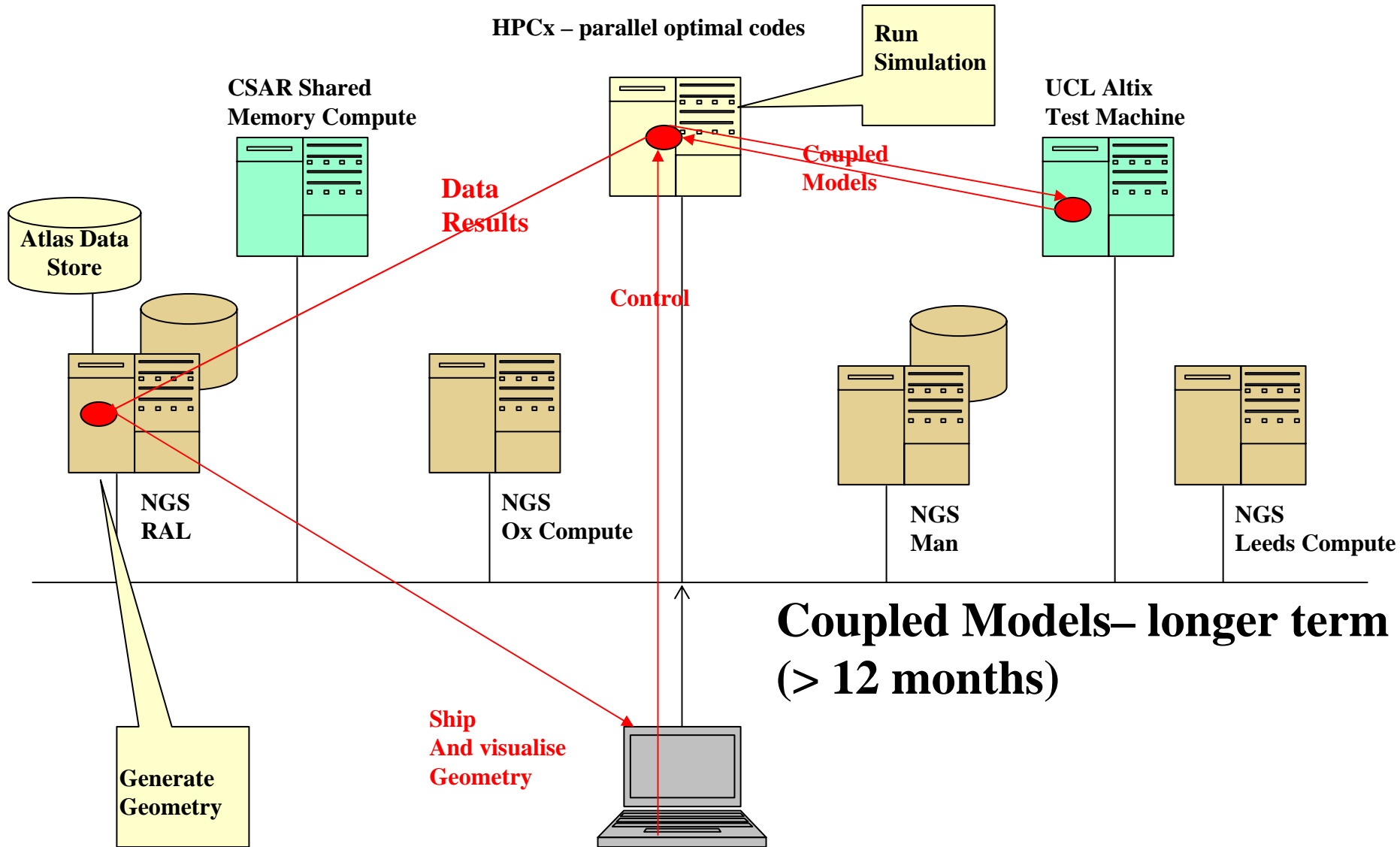
# To recap the technical challenge..

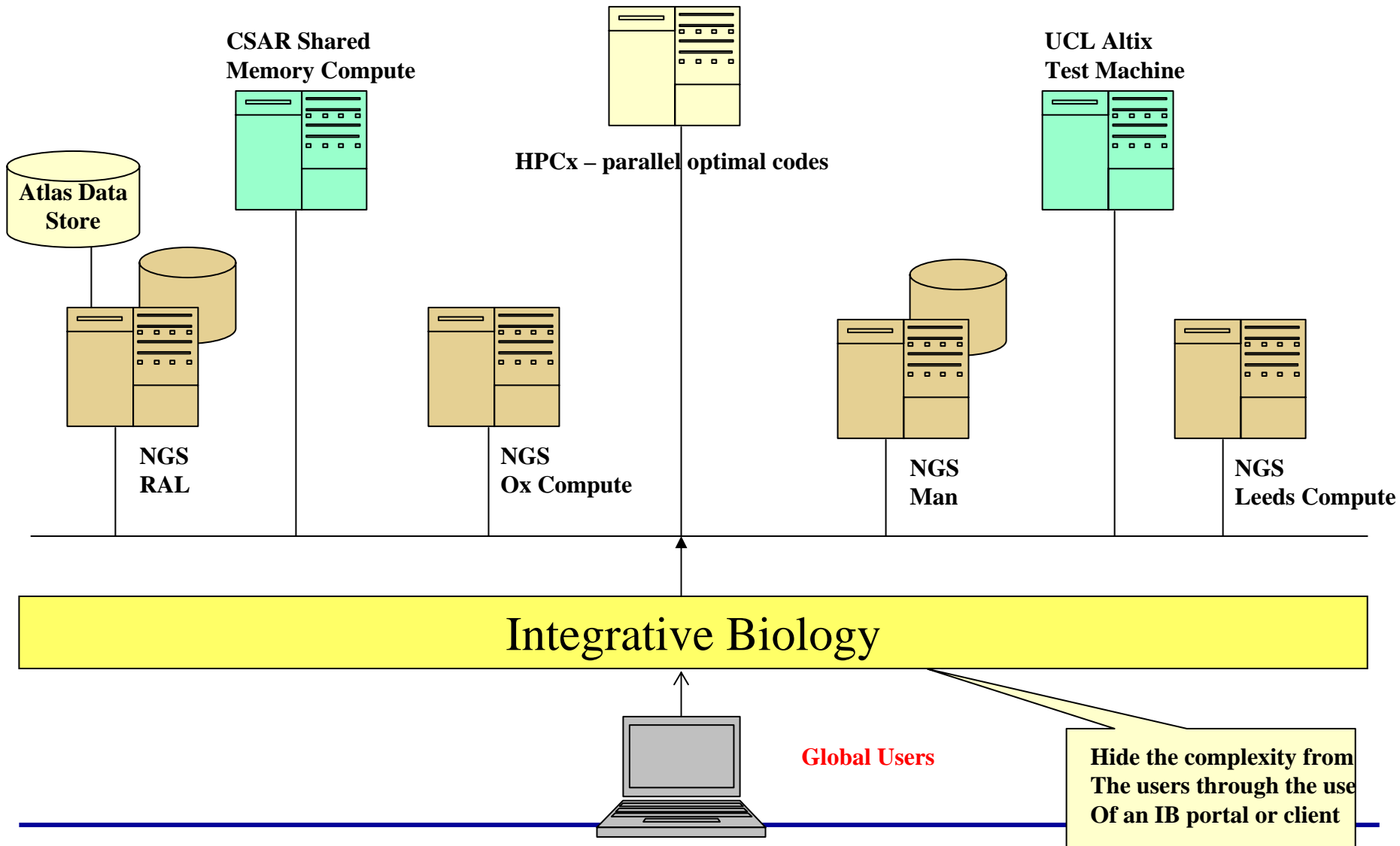


How do I use all this complex technology?  
How do I move from running my models on a personal machine?



**Global Users**





# Approach

- Pragmatic: enable users as quickly as possible to get full engagement using whatever tools are currently available *and straightforward to use*. Assist with HPCx, CSAR, NGS access
- Develop releasable solutions for scientists to use. Refined through feedback. Developed according to 6 monthly plans. More details from Damian Mac Randall
  - Release 1: Basic Portal, access to NGS and SRB data store
  - Release 2: Refined Portal, access to HPCx and CSAR, metadata editing, advanced visualisation, VRE
- Research new technical capabilities through demonstrators and prototypes

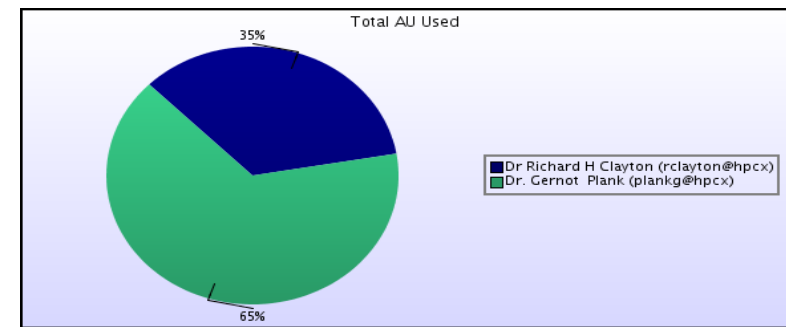
## Evolving Projects

- myGrid Best Practise (EPSRC) – 1 year 2005
- Reality Grid Best Practise (EPSRC) – 1 year 2005
- Sister Project for US travel (EPSRC) – 2 years till end IB
- IB VRE (JISC) – 2 years from April 2005
- Uklight – 2 years from April 2005

# Successes with national compute resources

## 1. HPCx

- Gernot Plank , Graz, Austria
  - Richard Clayton, Sheffield, UK
- Rob Blake, Chris Bradley, others  
Registered but not active at present



## 2. CSAR

- Richard Clayton, Sheffield, US
- Chris Bradley, Oxford



## 3. NGS

- Gernot Plank, Graz, Austria
- Blanca Rodriguez, Oxford



## IB VRE (Jisc)

- IB consortium has been awarded £300K from JISC to develop a Virtual Research Environment as a front-end to the IB system
- Will be built on the OGCE platform
- Will be undertaken in collaboration with Oxford University Computing Services (Mike Fraser and Matthew Dovey) and Rob Allan's group at CCLRC
- Start date March 2005 (planning)
- Recruitment process completed
- Requirements for initial prototype being refined at this workshop!

# We have demonstrated recently

## Science on national compute resources

- Richard Clayton – Cardiac Heart Modelling on the White Rose Grid, recently parallelised with Matlab interface and new visualisation techniques
- Gernot Plank, Utrecht – Heart Modelling on NGS via visualisation front end (user selected environment)
- Blanca Rodriguez (Thushka), Oxford – Heart Modelling in NGS via portal and visualisation via Meshalyser or Coolgraphics

# Demonstrations at this conference

## New technologies

- Workflow tools – demonstration of a simple workflow utilising the myGrid tools
- Advanced visualisation tools
- Metadata editor demonstration
- Computational Steering for coupled models

## 2005-6 Targets

- Release of portal and Meshalyser interfaces and services to new users
- Refinement, and extension of services through review including usability evaluation
- Advance move to HPCx and CSAR machines from portal
- Advance data management techniques
- Implement code management and release capability
- IB VRE development and implementation of new services
- Workflow development for IB through best practise project
- Advance US collaborative links through workshops and adoption of technology

# Summary

- User engagement well established
- Technology development incremental – evaluation and integration
- Any Questions?