Research Computing Facilities in Oxford

Oxford e-Research Centre

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Overview

- The OeRC

- Oxford Supercomputing Centre

- National Grid Service

- OxGrid, Oxford Campus Grid

The Oxford e-Research Centre

Dr David Wallom

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OeRC in the University

- A new research centre within the Mathematical, Physical and Life Sciences Division
- Wide remit to assist all departments to use innovative computational and information science in multidisciplinary collaborations
- (Will be) physically located within a new building on Parks Road

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The OeRC "hub" activities

Applications

Tools and Technologies

Infrastructure

Community

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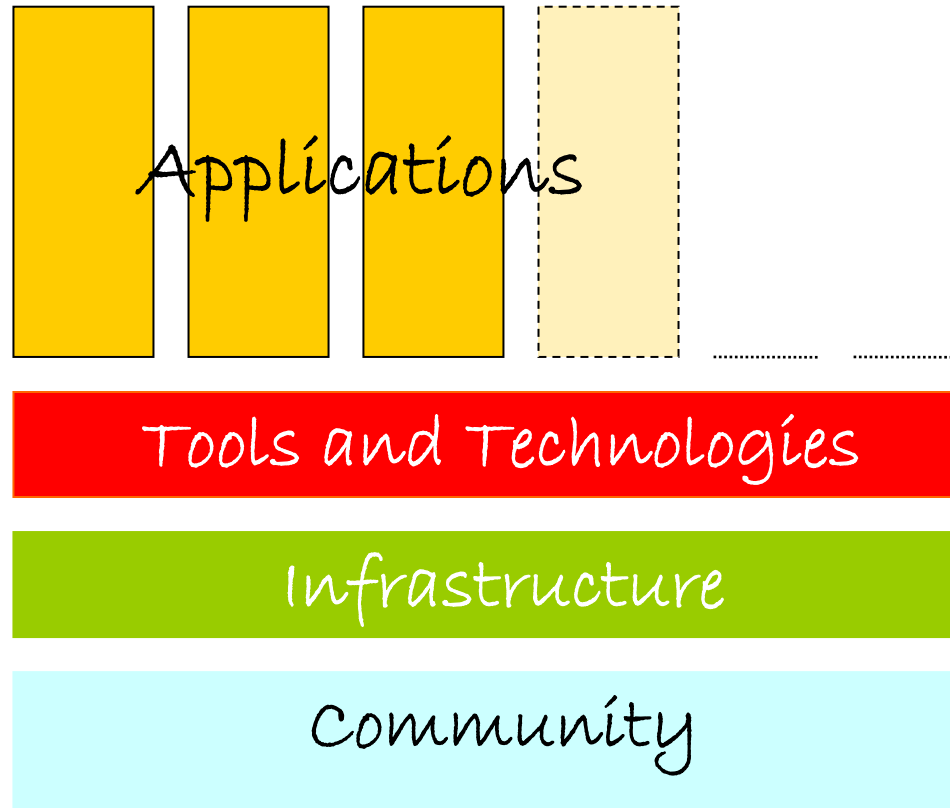
Applications

Extending the LamdaGrid "Optiputer" – with Angus Kirkland, Materials
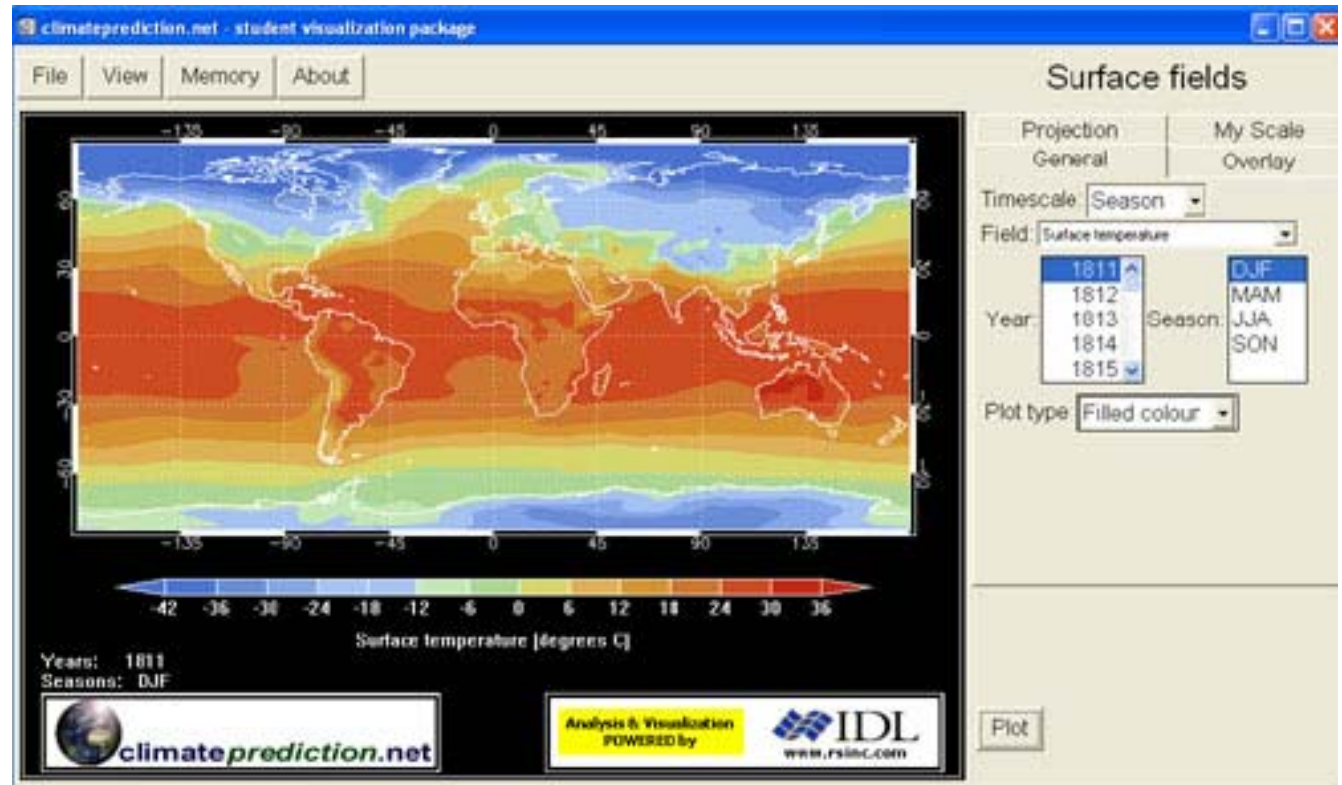

- World leading materials (Oxford) + biomedical (San Diego) researchers
- real-time data intensive
- compute, Lamda networks = high bandwidth, shared data storage, visualisation

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Applications

Climateprediction.net – Myles Allen, Atmospheric Physics

-Thanks to all of our participants - CPDN has hit a new milestone of 10 million model-years calculated.
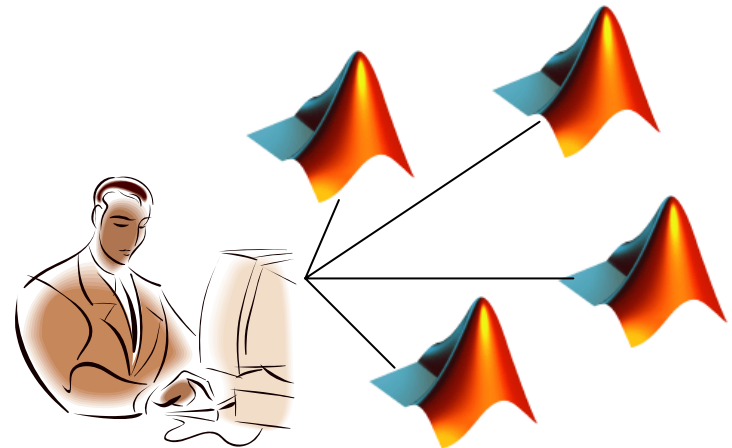
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Tools and Technologies

Harvesting and reusing from across e-Research projects

- For example, imaging has been a key part of earlier e-Science Projects such as eDiamond using tools such as MatLab

- Enabled a new project in collaboration with MathWorks to bring the toolboxes constructed to production quality

Matlab Distributed Toolbox +
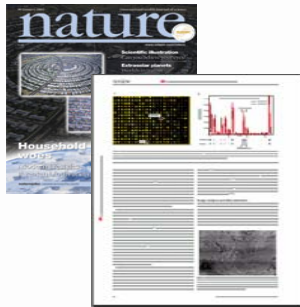
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Infrastructure

- Networks
  - Dark Fibre
- Services
  - OSC
  - NGS
  - OxGrid
- Institutional and other repositories
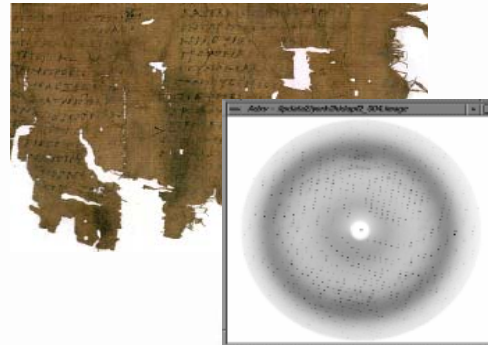- Access Grid video conferencing for improved collaboration

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Infrastructure

- Institutional repository

Literature

Images

Can only be produced by a large collaboration

- Researchers
- Computer scientists
- Technologists
- Librarians
- Service providers

Simulation data

Enabling the complete scholarly cycle

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Community

(Images courtesy of Bill Pulford CCLRC)

- Oxford/researchers
  - Building Bridges…..
  - e-Horizons
- Regional
  - CCLRC (Diamond, ISIS), Reading University
  - Schools & colleges, general public (Public Engagement in Science)
- National
  - UK e-Science core programme, eSI, NeSSC
- International
  - Harvard, Monash, UCSD
- Industry
  - IBM, Microsoft

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Some fundamental issues

e-Science Laboratory

Conclusions

- Engagement based on hub-and-spokes model for e-Research in Oxford

- OeRC engagement: locally, regionally, nationally, internationally, and with industry

- Very keen to engage with new areas of research in Oxford

- Please contact us through info@oerc.ox.ac.uk

OSC, a university computational resource

Dr Jon Lockley

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Oxford Supercomputing Centre

- Current Status:
  - Now formally part of OeRC
  - A member of OxGrid
  - Two new systems, "KONRAD" and "ZUSE" came on-line last summer
  - SRIF3 funding (£3m) in place but spending delayed (expected Autumn 2006)
  - Software license service is on-line

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How to submit jobs

- Users need to visit www.osc.ox.ac.uk to apply for an account

- Can then login directly **or use OxGrid account**

- **Which is best? Depends on relative needs for optimisation of code versus turn-around time.**

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How to pay for jobs

- We don't know!

- Service is currently free – fEC dictates that this cannot continue indefinitely

- The University continues to investigate how to recover costs

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Future Developments

- Increase the level of usage in areas other than MPLS division:
  - data mining
  - statistical analysis
- Strength areas other than floating-point performance
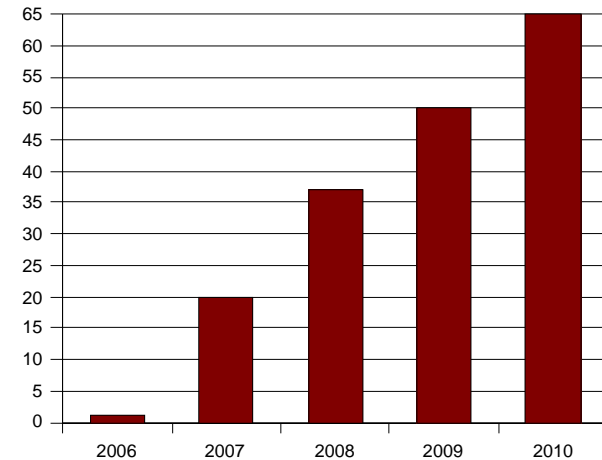 - HPC Storage
- Research new technologies

New Hardware

Number of Processing Cores

Year	Cores
2006	~150
2007	2000
2008	3000
2009	3000
2010	3000
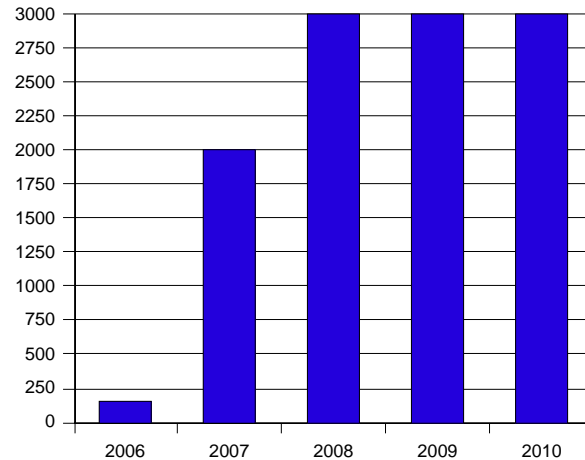
Relative Processing Power

Year	Power
2006	~1
2007	20
2008	37
2009	50
2010	65

- Mostly Linux clusters each with varying emphasis on "in-box" power and interconnect
- An SMP system

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The UK National Grid Service

Dr Steven Young

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National Grid Service

- NGS funded as part of the core e-Science programme (RCUK, EPSRC, JISC)
- 4 core sites (Oxford, RAL, Leeds, Manchester)
- NGS growing through addition of partners and affiliates.

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Oxford NGS Cluster

- Initial hardware delivered Oct 2003, initial service Apr 2004, in production Sep 2004.
  - 128 CPUs (64 dual 3GHz Xeons)
  - Myrinet interconnect
- New hardware arriving Oct 2006
  - Currently in tender

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How to submit jobs

- Grid interfaces only
  - Use the OxGrid interface.

- Apply for an NGS account
  - www.ngs.ac.uk/apply.html
  - OxGrid account will grant access to the Oxford NGS cluster. NGS account needed to access other NGS resources

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How to get help

- Local email: Currently ngs-help@oucs.ox.ac.uk
- NGS support email: Currently support@grid-support.ac.uk
- Other areas of NGS expertise
  - Database services, Oracle database hosting, OGSA-DAI
  - Data/storage services
  - Plans for visualization service

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OxGrid, A campus grid for the University of Oxford
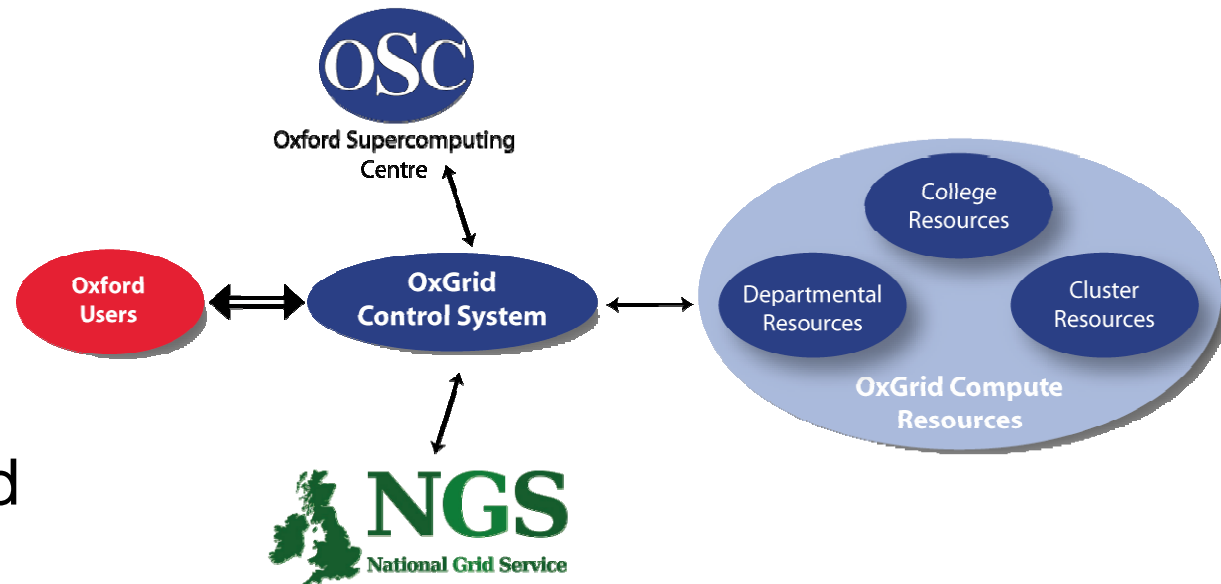
Dr David Wallom

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Why make a Campus Grid?

- Many computers throughout the University under-utilised:
  - Both PCs and Clusters are not normally fully utilised
- OxGrid: Develop and deploy Grid technology to gain;
  - Higher utilisation
  - Substantially increase the research computing power available
  - Provide data capacity to those groups unable to themselves

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OxGrid, The Idea

- Single submission point for Oxford users to shared and dedicated resources

- Seamless access to National Grid Service (NGS) and OSC for registered users

OSC
Oxford Supercomputing Centre

Oxford Users

OxGrid Control System

College Resources

Departmental Resources

Cluster Resources

OxGrid Compute Resources

NGS
National Grid Service

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OxGrid Resource Providers

- Current
  - All Users
    - Oxford NGS node
    - OUCS lecture rooms
    - Biochemistry
    - Particle Physics
  - Externally registered users
    - Oxford Supercomputing Centre (Zuse)
    - All of the NGS

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New Systems

- System additions within the next 3 months
  - Nuclear Physics (Cluster)
  - Theoretical Physics (Cluster)
  - Kellogg College (PCs running virtual machines)

- Other Department/College PC farms through virtual Linux technology

- Apple X-Grid clusters in OUCS & Physics

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Data Management

- Engagement of data as well as computationally intensive research groups
- Provide a remote store for those groups that cannot resource their own
- Use the Storage Resource Broker software from SDSC
- Distribute the client software as widely as possible

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Creating an SRB Data Grid

MCAT

SRB

SRB

SRB

SRB

SRB

SRB

Virtual Disk
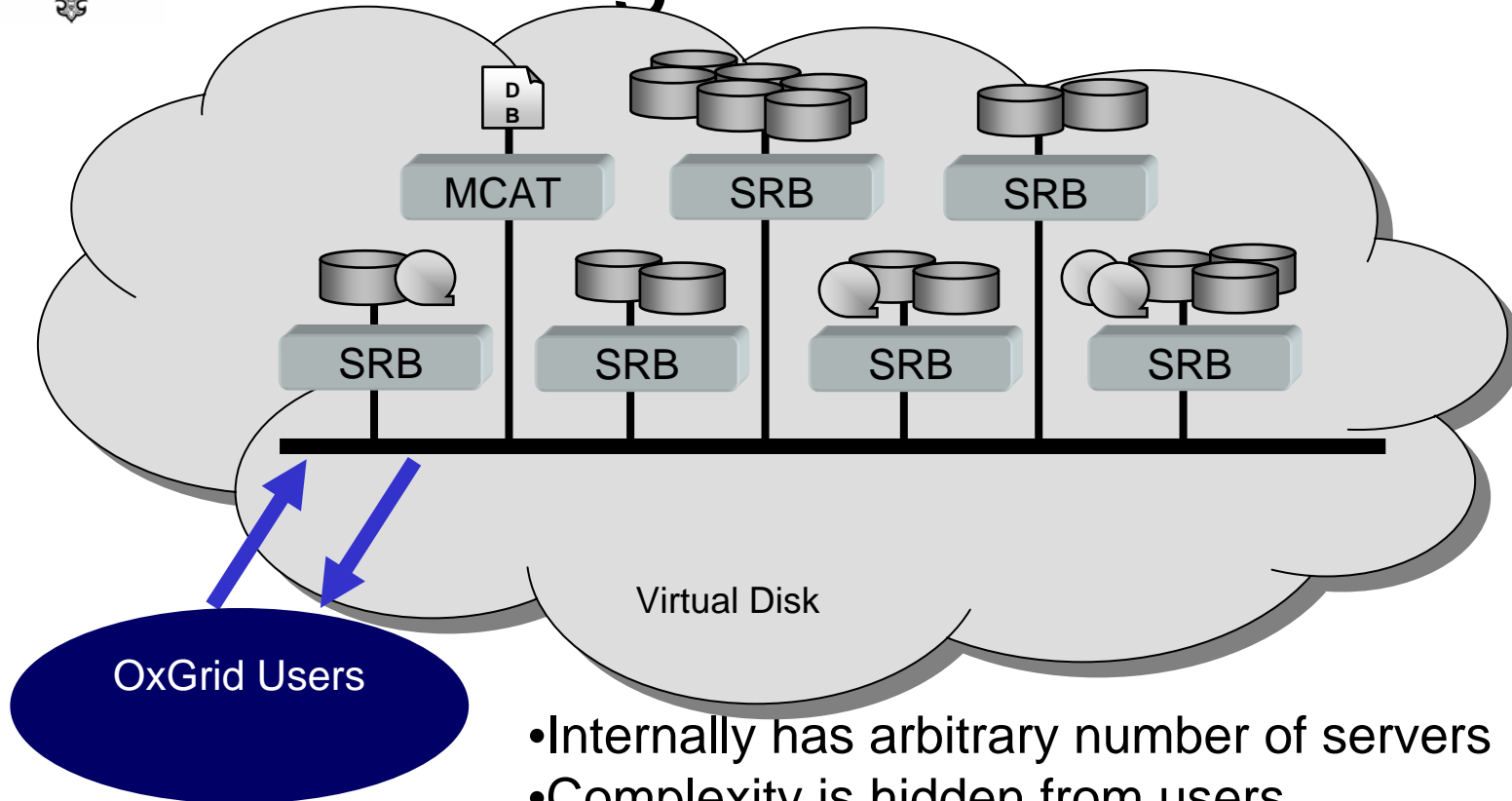
OxGrid Users

- Internally has arbitrary number of servers
- Complexity is hidden from users
- Command line, web-based and Java clients available for Linux/Unix/Windows

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How to get on OxGrid

- e-mail info@oerc.ox.ac.uk to register interest, we will then contact you!
- We will then ask you to;
  - Register for a UK e-Science digital certificate (http://ca.grid-support.ac.uk)
  - Supply University/"Herald" username
  - Supply an example of the work that you want to do so that we can create example application.
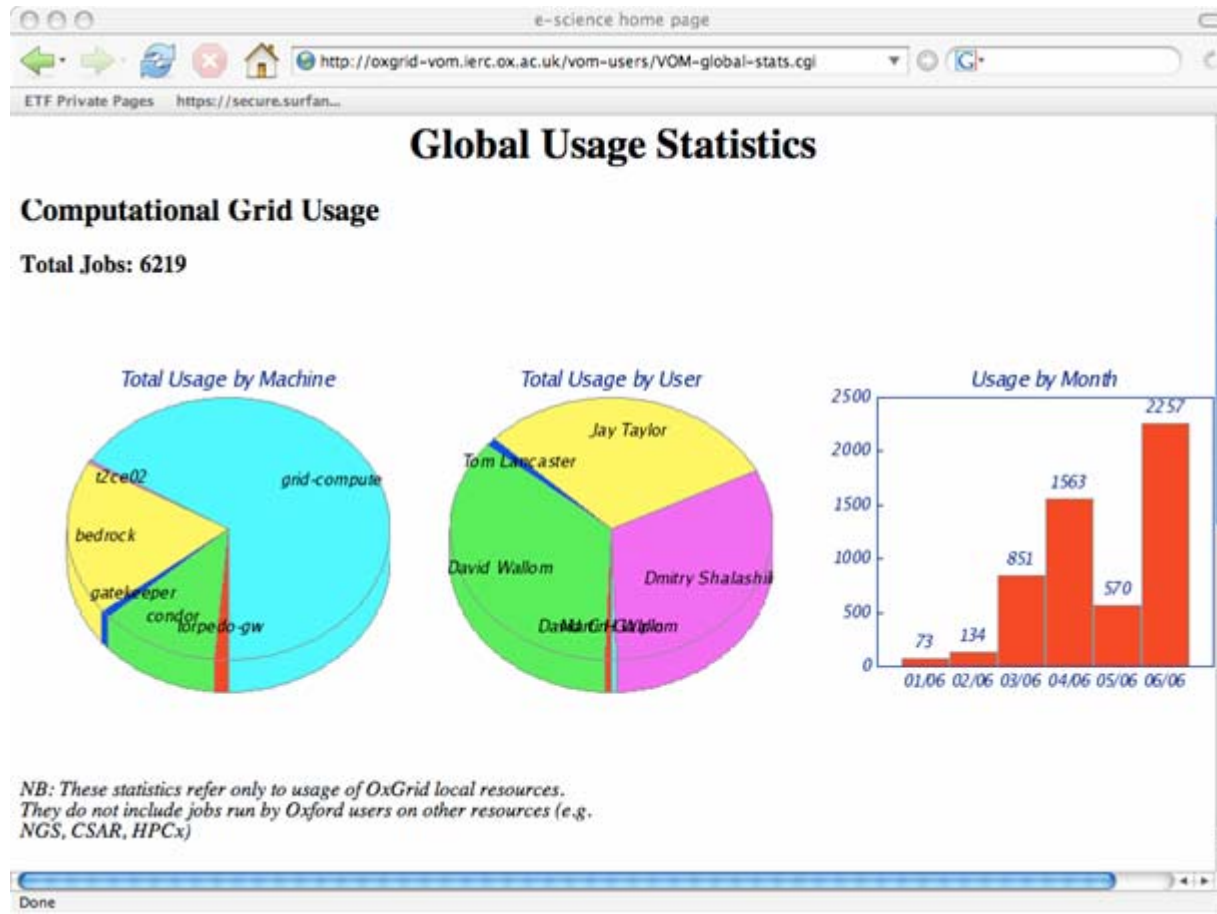- To make full use of the system we will also ask you to register for the NGS.

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Running Jobs on OxGrid

- Log onto central server
- Install application software (we can do this if necessary)
- Based on the example application we provided create wrapper submission script.
- Run jobs and wait for completion!
- Data is automatically stored in the DataGrid and can be retrieved to a local machine using installed tools

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Computational Usage accounting

Data Usage Accounting

OxGrid, Users

- Currently have registered users in the following groups
  - Chemistry
  - Inorganic Chemistry
  - Materials Science
  - Theoretical Chemistry
  - Statistics
  - Theoretical Physics
  - Nuclear Physics
  - Computational Biology
  - OUCS

Simulation of the quantum dynamics of correlated electrons in a laser field. OxGrid made serious computational power easily available and was crucial for making the simulating algorithm work. *Dr Dmitrii Shalashilin (Theoretical Chemistry)*
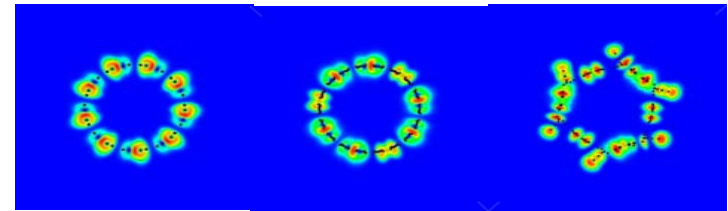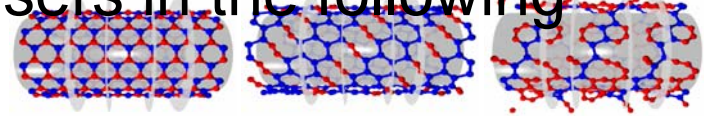
Orbitals and Electron Charge Distribution in Boron Nitride Nanostructures
Dr. Amanda Barnard, (Materials Science)

Molecular evolution of a large antigen gene family in African trypanosomes. OeRC/OxGrid has been key to my research and has allowed me to complete within a few weeks calculations which would have taken months to run on my desktop. *Dr Jay Taylor* (Statistics)

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Conclusions

- Large research computation and data facilities are available through the OeRC

- Users throughout the university are encouraged to make use of them!

- If you feel that e-Research tools and techniques could be useful to researchers in your departments make them contact us

- If you have resources that could be added to the campus grid then please contact us

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