The UKHEC Collaboration

← CLRC Daresbury Laboratory

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← Edinburgh Parallel Computing Centre (EPCC)

Manchester Research Centre for Computational Science (MRCCS) →

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The UKHEC Collaboration

- **In January 2000 EPSRC funded a 3 year core activity to track and disseminate information on international activities in computer architectures, software and programming tools and to promote good programming practice for the HEC community via workshops, seminars, reports and mentoring.**

- **The *UKHEC Collaboration* involves staff from**
  - **CLRC Daresbury Laboratory (2 FTEs),**
  - **Edinburgh Parallel Computing Centre (EPCC, 2 FTEs), and**
  - **Manchester Research Centre for Computational Science (MRCCS, 1 FTE)**

- **Information is provided in a Newsletter and via the Web site:**

  http://www.ukhec.ac.uk

- **A strategic collaboration between the three leading UK centres offering nation-wide high-end academic computing support.**

www.ukhec.ac.uk

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High-End Computing

- About
- Research
- Training
- Events
- Publications
- Contacts
- What's New
- Search

The aim of the UKHEC initiative is to investigate emerging areas of computing and to inform and provide advice to the user community in hardware and software developments, in new tools, in best practice code development and in data management.

There are three centres supported under the EPSRC co-ordinated High End Computing (HEC) programme. The centres are:

- EPCC - Edinburgh Parallel Computing Centre
- CLRC - Daresbury Laboratory
- MRCCS - Manchester Research Centre for Computational Science

In a related but separately-funded activity staff from these centres are also supporting e-Science projects throught the UK Grid Support Centre.

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UKHEC Programme

- Research
  - HEC Hardware and Software
  - Code Development, Maintenance and Porting
  - Good Practice in Data Management
  - Programming Tools and Environments
- Training
  - Training Courses
- Events
  - Seminars
- Publications
  - Newsletters
  - Technology Watch reports
  - Technical reports
  - Conference papers and talks

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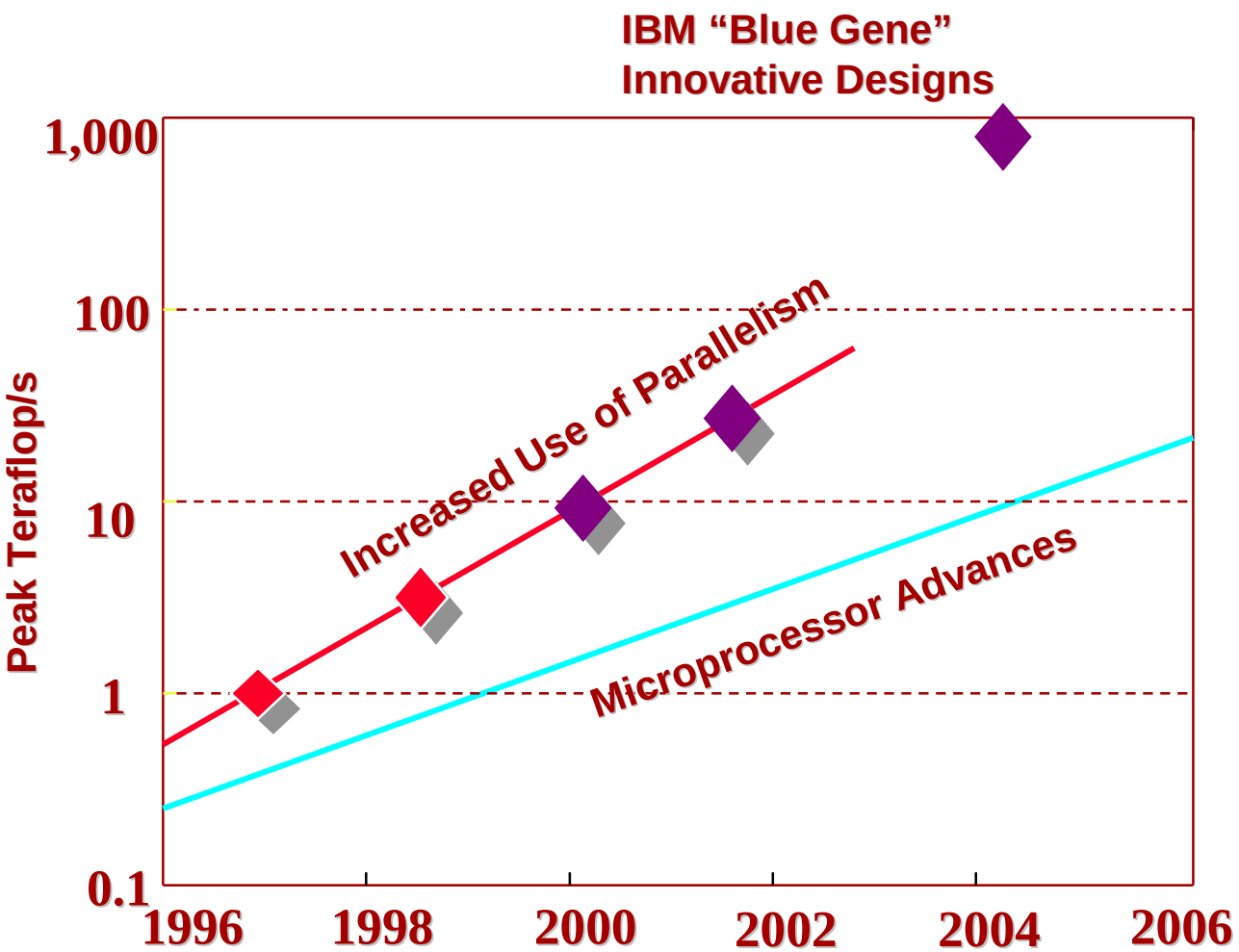
Dramatic Advances in HEC



MICROPROCESSORS

2 X increase in microprocessor speeds every 18 months ("Moores Law")

PARALLELISM

More and More processors being used on single problem

INNOVATIVE DESIGNS

Processors-in- memory

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Scientific Software Challenges

- **Peak Performance is skyrocketing**
  - **In past 10 years, peak performance has increased 100x; in next 5+ years, it will increase 1000x**
- **but ...**
  - **Efficiency has declined from 40-50% on the vector supercomputers of 1990s to as little as 5-10% on parallel supercomputers of today and may decrease further on future machines**
- **Research challenge is software**
  - **Scientific codes to model and simulate physical processes and systems**
  - **Computing and mathematical software to enable use of advanced computers for scientific applications**
  - **Continuing challenge as computer architectures undergo fundamental changes: *Algorithms that scale to thousands-millions processors***

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Key Topics

- Hardware: SMP/DM (ASCI) architectures, clusters (Beowulf)
- Software Development and QA Tools: faster development, maintenance and exploitation
- Languages (Java, C++, Fortran90): ease of use and performance
- Optimisation: need highest performance - can tools help ?
- Visualisation and VR: demonstrate VR capabilities for scientists
- Data Management: demonstrate fast storage and access for science apps.
- Grid computing environment: evaluation and use of Globus, coordination of e-Science activities between centres
- Standards: portability and longer code lifetime
- OpenMP/ MPI Programming: optimize for heterogeneous architectures

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Highlight #1:
GUIs for Scientific Computing

Applications: ease-of-use, computational steering & 'productisation'

- **Technical Report & Workshop, 4th July 2002, Daresbury**
- **What the issues in building a GUI ?**
  - ease of download, build, use and learning
  - ease/speed for manipulation of GUI objects and 3D graphics
  - ability to link to native code (Fortran, C)
  - quality of support for multi-thread applications
  - choice of toolkits
  - choice of open-source solutions
  - can they be distributed as part of a package ?
  - portability, cross-platform aspects

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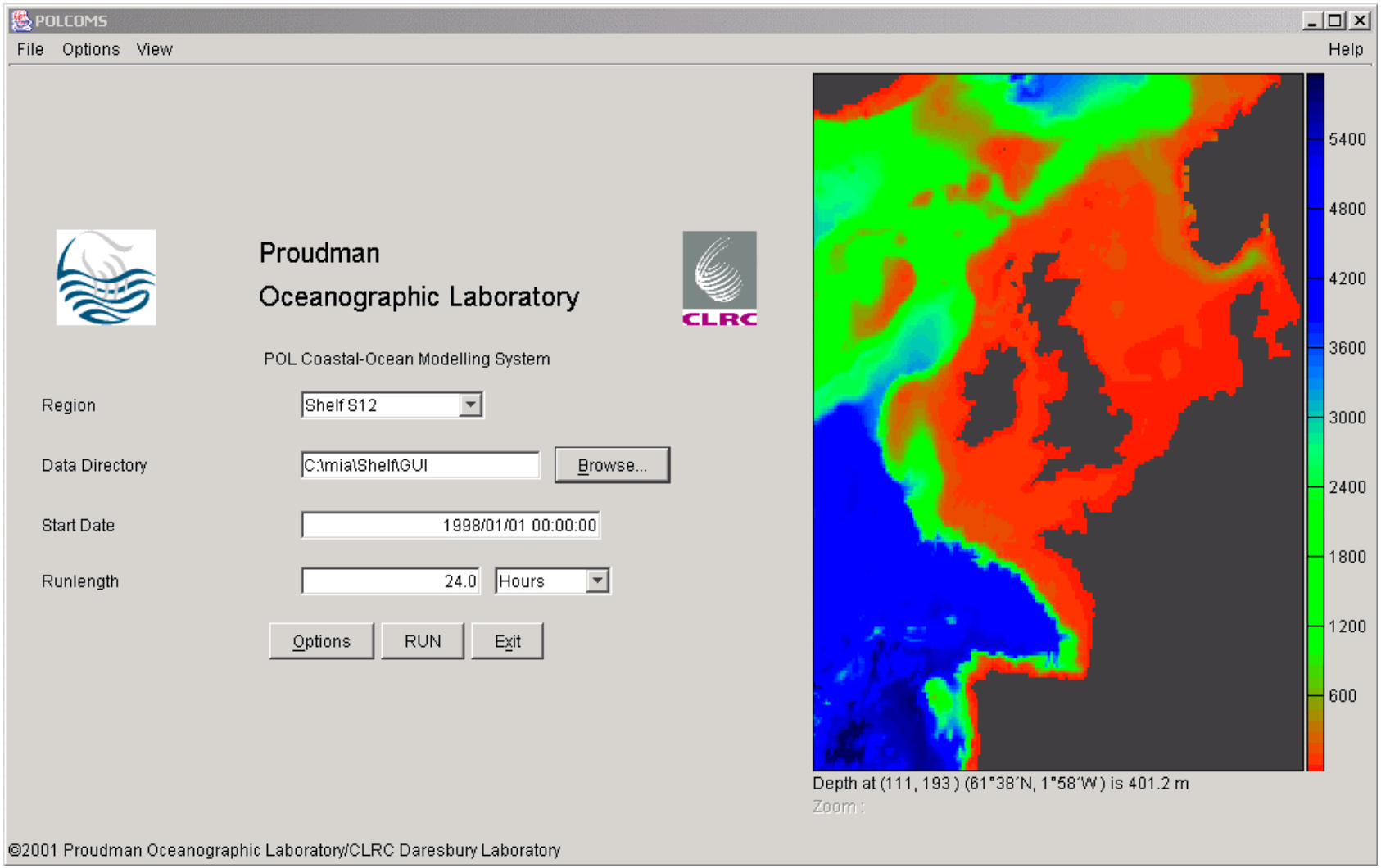
POLCOMS Java GUI



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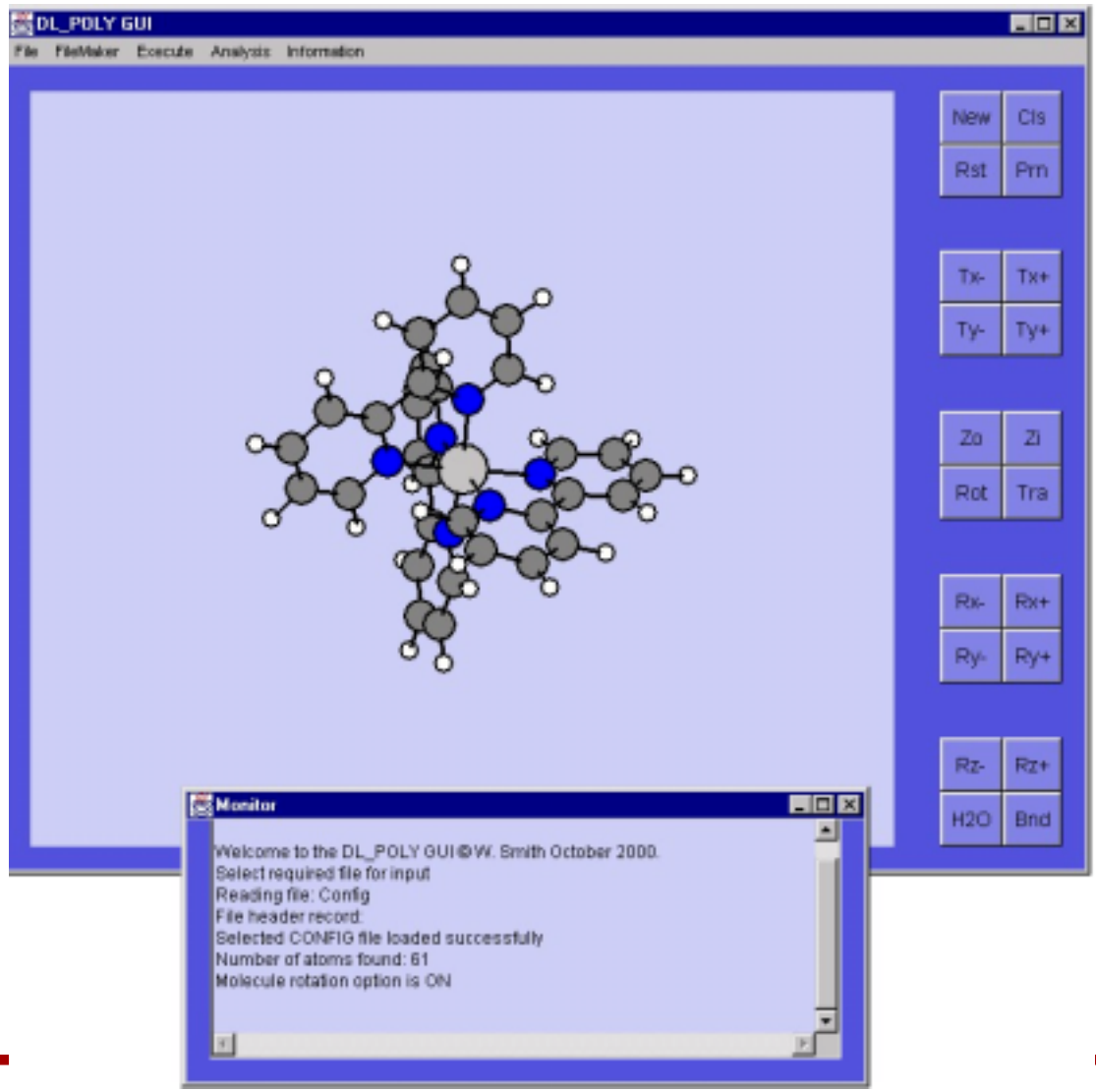
DL_POLY Java GUI



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Highlight #2:
Application Development

More robust, portable and easily maintained applications

Technical reports:

Data Distribution, Migration and Replication on a cc-NUMA Architecture

Applied Numerical Libraries for Parallel Software

Portable Application Compilation and Building for Fortran 90

Investigating use of XML in Java application codes

Java for High Performance Computing.

Data Management Tools for High Performance Computing Applications

Training course:

Programming Shared Memory Systems

8th November 2002 - University of Edinburgh

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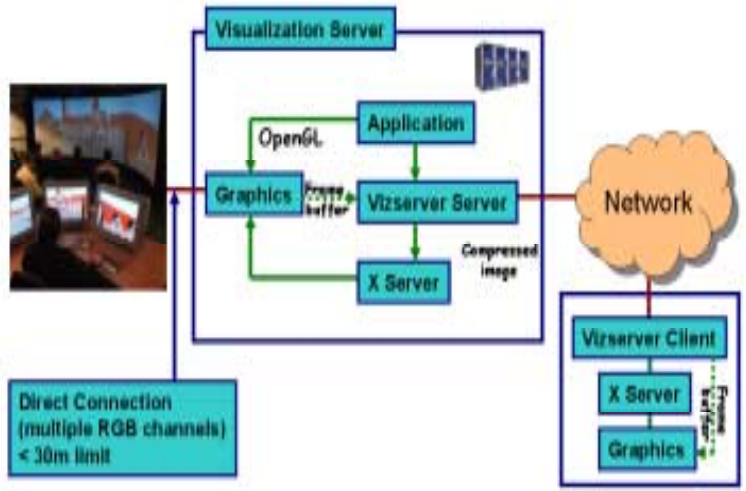
Highlight #3a:
Visualization for Insight

Analysis of scientific data for new insight



Scientific Application of OpenGL Vizserver within High Performance Computing

Reports:

Scientific Applications of Visualization, Virtual Reality and High Performance Visualization Computers

Scientific Examples of Virtual Reality and Visualization Applications

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Highlight #3b:
Visualization for Insight

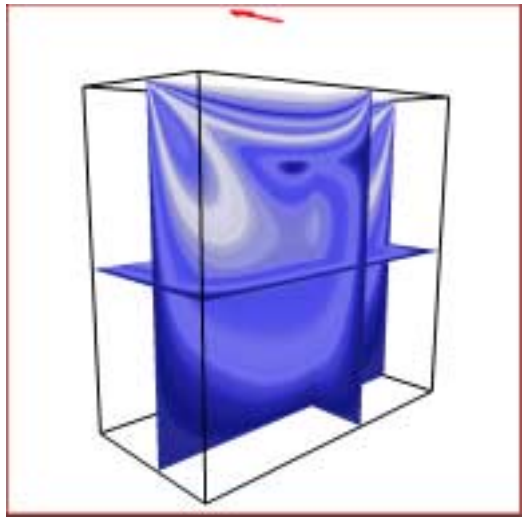
Analysis of scientific data for new insight

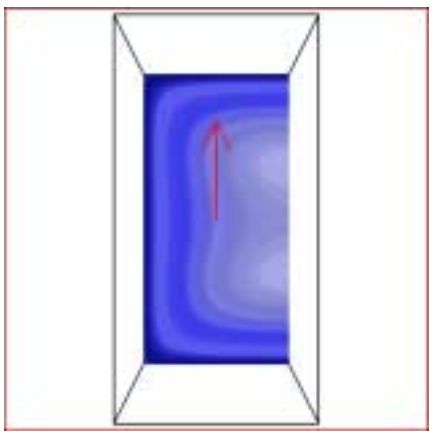
Visualizing

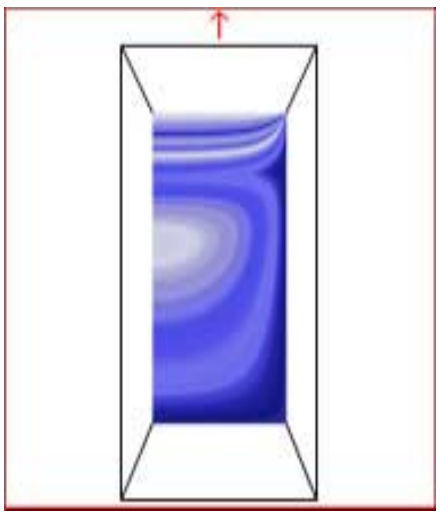
Large Parallel

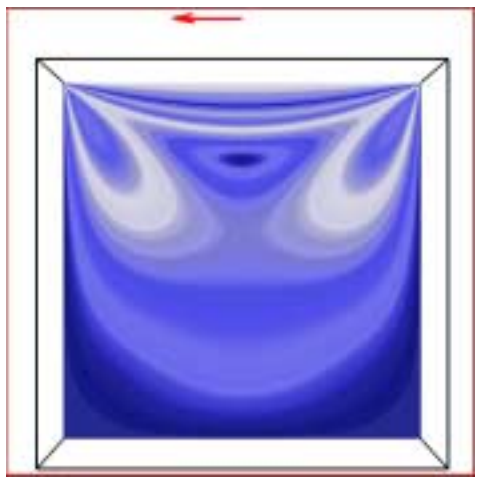
Finite Element

Simulations









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Highlight #4:
Grid Developments

Enable flexible and easy access to local and national facilities

- Single point of login
- Internet security standards and authentication
- Remote access to local and national facilities
- Integration of compute resources, data centres and experimental instruments
- Development of problem solving environments

– **Consultancy and technical input into many e-Science projects**

– **Partners all established e-Science centres and collaborate in UK Grid Support Centre and Access Grid**

– **Seminar on GRID Portals and Resource Discovery,** 4th July 2002, CLRC Rutherford Appleton Laboratory

– **Grid Seminar describing commercial middleware and solutions,** 30th November 2001, CLRC Daresbury Laboratory

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Highlight #5:
Cost Effective Visualization

Visualization for Cost Effective Insight

The Future of High Performance Visualization – Does it Lie With Consumer Graphics Hardware?

VS.

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Forthcoming Seminar #1

Data Management for High End Computing

- **Focuses on the challenges and methodologies of Data Management for scientific codes**
- **Examples from a range of scientific disciplines**
- **Draw out similarities and commonalities so that different user communities can benefit from one another**

Friday 10th January 2003
CLRC Rutherford Appleton Laboratory

Dr. John Ashby

J.V.Ashby@rl.ac.uk

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Forthcoming Seminar #2

Advances in Visualization For HPC

- **Keynote speaker: Chuck Hansen from University of Utah**

To be held early February 2003

Manchester Computing

Date and full details to be announced

See www.ukhec.ac.uk

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The Future: HPC Systems - Access and Efficiency

Context: HPC(X) and UK e-Science Environment

1) Continue and Extend Technology watch brief

- **evaluate new methodology, architectures and programming standards (working with tools fora, international research groups and vendors)**
- **target new communities (e.g. other RCs)**

2) The Computational Grid and HEC Applications

- **outreach: extend Grid-based applications to High End facilities**
- **investigate distributed computing algorithms to provide highly scalable "loosely coupled" methods for HEC systems**

3) Work with Application Developers

- **extend dissemination brief with more focus on applications by working directly with code developers to evaluate new techniques**

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