Application Trends on HPCx

Providing a World-Class Service for World-Class Research

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Aim of the talk

- HPCx has been in operation for almost four years
- Large range of statistical data generated during this time
  - Subject areas
  - Codes
  - Length of jobs
  - Size of jobs (processors)
  - Discounts
- Aim is to review some of the more interesting observable trends
System trends

- Undergone/going four technology upgrades, three different types of system / processor
- Phase 1 (Dec 2002 – June 2004)
  - 3.4 Tflops on Linpack
  - 1280 power4 processors, 40 p690 cabinets
- Phase 2 (July 2004 – Oct 2005)
  - 6.2 Tflops on Linpack
  - 1600 power4+ processors, 50 p690+ cabinets
- Phase 2a (Nov 2005 - Oct 2006)
  - 7.4 Tflops on Linpack
  - 1536 power5 processors, 96 p575 nodes
- Phase 3 (Nov 2006 – Dec 2008)
  - Target 12 TFlops/s on Linpack
  - XX power 5 processors
Performance trends – acceptance tests

- AIMPRO (128 processors): 2.1 times faster
- CASTEP (128 processors): 3.4 times faster
- DL_POLY (128 processors): 2.3 times faster
- H2MOL (496 processors): 2.3 times faster
- PCHAN (512 processors): 2.4 times faster
Usage trends - available AUs / average usage

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• Historically, HPC has played an important role in computational ‘grand challenge’ science

• Grand challenge science
  - Projects which are almost too difficult to investigate using current computer technology

• By definition, grand challenge science requires high performance computers
  - Need vast amounts of memory and / or processing power

• The UK’s national HPC resources have supported this science since the early 80s
The report *Research Requirements for High Performance Computing* identified the following grand challenge areas in 1992:

- Climate modelling
- Astrophysics
- Quantum chromodynamics
- Materials science
- Structural engineering
- Computational fluid dynamics
- Human systems
• Utilisation figures for the UK’s National HPC resource in 1996 - the Cray T3D in Edinburgh
T3D 1996 vs HPCx 2003

PPARC funded, now utilising other resources e.g. QCDOC

- Chemistry and Materials
- Engineering
- Environment
- Physics/Atomic Physics
- Biology/Life Sci
- Human Systems
- QCD
- Cosmology

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Application area trends

Materials
Environment
Engineering
Physics
External
Life Sciences
Chemistry

Percentage Usage

2003
2004
2005
2006
Application area trends

• The largest users of the system are Materials and Chemistry
• However over the lifetime of the service we have seen
  - An increase in engineering
  - An increase in the environment
  - Life science projects joining the service
  - Some external industrial customers joining the service
• HPCx now supports a broader range of subject areas
Most heavily used codes

- Start of service

- Now - 2006
Job size trends - capability science

- Science still drives HPC requirements within the UK
- Focus of current HPC resources is to facilitate world-class science
  - Through capability science
- Specifically
  - Science that uses a significant fraction of our resource, eg 512+ CPUs
Job sizes - start of service

- Job sizes dominated by 128-256 jobs (mainly 128)
Job size trends

- 2003
- 2006

Percentage
Capability job size trends

AUs utilised

Consortium 1
Consortium 2
Consortium 3
Consortium 4
Consortium 5
Job size trends

- Significant shift from 128-255 processor jobs to larger jobs
  - 256-511 and > 512
- Capability jobs
  - Usage within a consortium various significantly across time
- 47 consortia have run capability job(s) at some time
Usage by region

Scotland: 2%
Northern Ireland: 10%
England, North West: 9%
Wales: 1%
England, West Midlands: 0.3%
England, South West: 16%
England, North East: 4%
England, Yorkshire: 1%
England, East Midlands: 1%
England, East Anglia: 13%
England, London: 14.3%
England, South East: 18%
Heaviest users (> 2%)

- University of Edinburgh, 2%
- University of Durham, 3%
- University of Bristol, 4%
- Imperial College, 6%
- University of Kent, 6%
- CCLRC, 9%
- University of Southampton, 9%
- Queen's University Belfast, 10%
- University of Reading, 2%
- University of Cambridge, 13%
- University College London, 12%
- Other Universities, 21%
Heaviest users (> 2%)

- e06, Prof Paul Madden: 20%
- e01, Dr Gary Coleman: 5%
- e02, Dr Patrick Briddon: 4%
- e03, Prof Ken Taylor: 6%
- e04, Prof Jonathan Tennyson: 7%
- e05, Prof Richard Catlow: 19%
- n02, Prof Alan Thorpe: 7%
- n03, Prof John P Brodholt: 4%
- e14, Prof Neil Sandham: 2%
- e20, Dr Ken Badcock: 3%
- n01, Dr David Webb: 6%
- Other Consortia: 14%
Usage by funding body

- PPARC
- NERC
- External
- EPSRC
- BBSRC

Number of AUs

Jan - Mar 2003
Jun 2003
Sep 2003
Dec 2003
Jan - Mar 2004
Jun 2004
Sep 2004
Dec 2004
Jan - Mar 2005
Jun 2005
Sep 2005
Dec 2005
Jan - Mar 2006
Jun 2006
Sep 2006
Dec 2006
Conclusions

• HPCx has been running successfully for 4 years
• Range of application areas has increased across the service
  - Increase in environment, life science and commercial usage
• Average job size has increased, as has overall capability usage
• Users are spread across the country
  - Heaviest use is from the south east of England
  - Heaviest use is from the University of Cambridge

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