Early Experiences with HECToR

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HECToR

- Latest high-end computing service for UK
  - managed by EPSRC on behalf of RC-UK
  - funded by EPSRC, NERC & BBSRC
  - will run from 2007-2013

- Objective:
  - to provide a service to the academic community enabling it to do true capability science

- Partners:
  - Service Provision: UoE HPCx Ltd
    - hardware hosting and maintenance
    - user services, help desk etc
  - Hardware: Cray Inc
  - Computational Science & Engineering Support (CSE): NAG Ltd
Overview of the CSE Service

- Partnership with HECToR user community to assist in deriving maximum benefit from the hardware:
  - Initial assessment of project suitability
  - Training
  - Documentation, case studies, FAQs
  - Help desk
  - Assistance with porting, performance tuning and optimisation of codes
  - 60% of resources dedicated to specific users, research groups or consortia

- NAG brings expertise in
  - Numerical Analysis and statistics
  - Software engineering

- General brief to help to improve scientific software in the UK
Hardware Solution

- Phase 1 (September 2007)
  - Cray XT4 (63 Tflops)
    - 5664 dual core Opterons
    - 33.2 TB memory
    - SeaStar2 Interconnect
  - BlackWidow Vector (2 Tflops)
    - after 9 months
  - 576 TB direct storage (rising to 934 TB)

- Phase 2 (2009)
  - Cray ??? (c 250 Tflops)
    - quad core ‘Barcelona’
    - faster interconnect

- Phase 3 (2011)
  - > 500 Tflops

Results Matter. Trust NAG.
HECToR Early Users

- Early user service started September 2007
  - Material Science
    - AIMPRO, VASP
  - Engineering
    - PCHAN
  - Chemistry/Biochemistry
    - AMBER, NAMD, PMEND, DLPOLY
  - Environmental Science
    - UM, NEMO
  - Physics
    - HELIUM, CENTORI, GS2, ORB5, QCD codes

- Next major group: “HECToR Capability Challenge” December 2007
Issue 1: Data Storage / Transport / Analysis

- 576 TB of storage initially
  - of which 40 TB can be backed-up
  - maximum 9 GB/s read-write bandwidth
  - disk-to-disk copy of 250TB would take at least 51 hours

- HECToR connected to SuperJanet
  - 10 GB/s backbone

- Example: Unified Model
  - typical output data O(10GB)

- Some scope for post-processing on HECToR
  - mainly batch environment
  - no support for visualisation, computational steering etc.
Visual Analytics

- Combine statistical & visualisation techniques
  - identify key characteristics of data set
  - understand those characteristics through visualisation
- ADVISE: UK TSB-funded research project
  - NAG / VSN / University of Leeds
- User community
  - pharmaceutical / environmental science / engineering / medicine
  - data sets up to 1.5GB
- Service-oriented technology
  - web services, distributed visualisation
  - ‘intelligent’ datatypes supporting distributed, out-of-core storage
- First prototype implemented
Issue 2: Code Management

- Typical user code
  - Implemented in Fortran
  - Uses MPI for parallelism
  - Written by generations of graduate students and PDRAs

- NAG’s role in HECToR
  - Advise on good software-engineering practices
  - Help with optimisation, tuning and scaling
  - Preserve performance across hardware upgrades
  - Make better use of standard software components and libraries
Hardware Upgrades

- HECToR Phase 1: 2.8GHz dual-core opterons
  - SSE via 64bit FPU
- HECToR Phase 2: 2.6GHz (?) quad-core “barcelona”
  - SSE via improved 128bit FPU

- AMD Core Math Library (ACML)
  - developed in collaboration with NAG
  - includes LAPACK, FFTs, RNGs, …
  - many kernels coded in assembler and tuned for particular chips

- To maximise performance many assembler kernels in ACML have been (laboriously!) re-written
  - better choice of instruction to reduce latencies
  - re-ordering code to ensure instructions done in parallel
Issue 3: Developments in Hardware

- Not HECToR-specific but relevant to anybody developing scientific codes
- Multi-core / many-core / GPGPUs / FPGAs etc
  - performance per watt becoming important
  - disruptive technology, codes will need to be rewritten
  - need for software that adapts to host environment
  - golden opportunity to introduce new algorithms and computational techniques
Conclusions

- HECToR will be a major tool for “high end” UK Science for the next six years
- The ability to store and transport data is becoming a bigger restriction than the availability of computational resources
- The wide availability of good-quality components can help insulate users against changes in hardware in short term
- Many codes may soon need to be re-written to take account of architectural changes …
- … making this a perfect time to incorporate radically new algorithms and computational techniques