CSE Update

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CSE Service: Overview

- Core Support
  - Technical assessments
  - Helpdesk queries
  - Assistance with porting/tuning etc
- Training
- Distributed Support
  - Dedicated resources for projects

Training

- Train HECToR users and researchers under BBSRC, EPSRC & NERC remits
- Most training happens at user sites
  - Bath, Belfast, Birmingham, Bristol, Cambridge, Exeter, Imperial, Leeds, Nottingham, Oxford, Southampton, Warwick
  - Summer schools, doctoral training programmes, training for grant holders ...
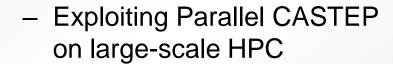- Over 800 attendees so far

Current Courses

- **HECToR Specific**
  - Introduction to HECToR
  - Programming the X2 Vector System
- **Programming**
  - Fortran 95
  - Parallel Programming with MPI
  - OpenMP
  - Parallel I/O
- **Application Specific**
  - DL_POLY

  - Exploiting Parallel CASTEP on large-scale HPC
- **Other**
  - Debugging Profiling and Optimisation
  - Multicore
  - Core Algorithms for High Performance Scientific Computing
  - Best Practice in HPC Software Development
  - Scientific Visualisation

Distributed CSE

- Dedicated support for specific codes
- Awarded by an independent panel
- Current status
  - 23 projects completed
  - 18 projects running
  - 7 projects waiting to start
- 558 months (46.5 years!) effort allocated to date
- Next deadline for proposals December 6th
  - New time limit of one year (elapsed)

DCSE Example: CASINO

- Quantum Monte-Carlo calculations on condensed matter
- DCSE delivered
    - better memory utilisation using shared data between tasks on the same processor
    - accelerated computation speed (60-80%) via second level parallelism
    - faster input of large data sets
- Benefits
    - CASINO able to exploit larger machines (JaguarPF, HECToR 2b) to solve bigger problems
    - 12m AU savings in one year on HECToR
    - Code improvements fed back to developers

DCSE Example: CP2K

- Atomistic and molecular simulations of solid state, liquid, molecular and biological systems

- DCSE delivered
  - improved MPI communications and load balancing (particularly for FFTs)
  - 30% speedup in typical cases (300% in extreme cases)
  - improved scaling (factor of 8 in some cases)

- Benefits
  - Researchers now able to routinely model cells with over 1000 atoms
  - 4.5m AU savings for one year on HECToR
  - Code improvements fed back to developers

DCSE Example: DL_POLY_3

- Molecular dynamics code
- DCSE Delivered
  - improved I/O by large-scale data reorganisation and by parallelisation
  - improved scaling to thousands of cores for real examples
  - reduced storage requirements for output files (typically by a factor of 3)
- Benefits
  - 20x improvement in performance made it feasible to use DL_POLY_3 to study eggshell formation
  - Code improvements fed back to developers

Summary

- Core CSE team available to assist with migration issues 2a→2b →3
- Training proving popular
  - suggestions for venues, tailored courses, application codes etc. welcome
- DCSE very successful
  - has enabled improved science
  - has saved resources

Questions?