CSE Update

Mike Dewar NAG Ltd





CSE Service: Overview

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





Core CSE Example: DG-DES

- Benchmarked original code with Pathscale and PGI
- Identified best compiler options
- Profiled code, wrote timing routines
- Reordered and restructured code to improve performance
- Investigated scaling characteristics
- Overall, produced a 70% performance improvement
- <u>http://www.hector.ac.uk/cse/reports/DG-DES.pdf</u>
 Image: Constant of the second se

Distributed CSE Status

- Six calls, five panel meetings
- 20 projects currently running
- 1 project completed
- More than 20 years of effort allocated so far
- <u>http://www.hector.ac.uk/cse/distributedcse</u>





Codes Benefiting from DCSE

- ACPIM
- CABARET
- CASINO
- CASTEP
- ChemShell
- CITCOM
- Code_Saturne
- CP2K

- CRYSTAL
- DL_POLY_3
- EBL
- GAMESS-UK
- GLOMAP
- HELIUM
- ICOM
- Incompact3d

- •LEM
- •MRBV
- •NEMO
- •OpenFoam
- •PRMAT
- •SS3F
- •SWT
- •WRF





Training

- Offering at least 76 days training per year
- Training at user institutions:
 - Bath, Birmingham, Imperial, Southampton, Bristol
 - Coming soon: Warwick, Manchester, Cambridge, Belfast
- Most popular courses:
 - Parallel Programming with MPI
 - OpenMP & Mixed Mode Programming
 - Introduction to Fortran 95
- Customised courses for individual groups
- <u>http://www.hector.ac.uk/cse/training</u>





CSE Support for Phase 2

- Advice
 - <u>http://www.hector.ac.uk/cse/documentation/Phase2</u>
- Assistance via helpdesk
 - benchmarking, porting, tuning
- Training & Workshops
 - in conjunction with Cray CoE
- DCSE Support
 - applications related to migration to phase 2 get preference in next two calls
 - deadlines 15 June & 15 September





Summary

- CSE Team provides
 - reactive support via helpdesk
 - dedicated support via Distributed CSE
 - training
 - assistance with migration to phase 2
- CSE staff happy to visit you to discuss any of the above



