

# HECToR DCSE Workshop

Mike Dewar  
NAG Ltd



# DCSE Application Areas

- Hartree-Fock / density functional theory
- Atomistic and molecular dynamics simulations
- Quantum mechanics with ab initio models
- R-matrix theory
- DNS of turbulent multiphase combustion
- Multi-scale LES of fractal objects
- LES of aircraft noise
- Non-hydrostatic ocean modelling
- Quasigeostrophic ocean modelling
- Surface water / sediment modelling
- Climate and seasonal forecasting
- Global atmospheric studies
- Plasma simulation
- Statistics for bioscience
- Structural modelling

# HECToR Distributed CSE Evaluations

- CSE Performance Working Group
  - EPSRC, Cray, Rolls Royce, HECToR User, NAG
- Scores completed projects on extent to which objectives met, and “impact”:
  - CASTEP: Improved efficiency and scalability, saving £2M in HECToR resource
  - DL\_POLY\_3: Implemented parallel I/O leading to 20x speed-up in application studying egg-shell formation, making running on HECToR feasible
  - CARP: Time to simulate 1s of human heartbeat reduced from 75 minutes to 5 minutes, opening up possibilities of use in clinical applications
- 23 projects evaluated to date:
  - Average Scores 4.7/5, 4.5/5



# Common Themes

- Mixed mode parallelism – OpenMP / MPI
- Structured data decompositions, e.g. FFTs
- Unstructured data decompositions – improving load balancing/communications
- I/O – MPI I/O and dedicated I/O nodes
- Inter node communications – optimising MPI point-to-points and collectives