Experience with the Cray XT Service at Edinburgh

Dr Mark Parsons
Commercial Director, EPCC
m.parsons@epcc.ed.ac.uk
+44 131 650 5022

EPCC

- The University of Edinburgh founded EPCC in 1990 to act as the focus for its interests in parallel computing
- Today, EPCC is a key European supercomputing centre
  - 70 permanent staff
  - Managing all UK national HPC facilities
  - Work 50:50 academia and industry
- In 2007 we won the contract to host the UK National Service HPC service - HECToR

The HECToR Service

- HECToR: **H**igh **E**nd **C**omputing **T**erascale **R**esource
- Procured for UK scientists by Engineering and Physical Sciences Research Council – EPSRC
- Competitive process involving three procurements
  - Hardware – *Cray Inc*
  - Accommodation and Management – *UoE HPCx LTD*
  - Computational Science and Engineering Support – *NAG*
- EPCC won the A&M procurement through its company – UoE HPCx Ltd
- HECToR is located at The University of Edinburgh at our custom built Advanced Computing Facility

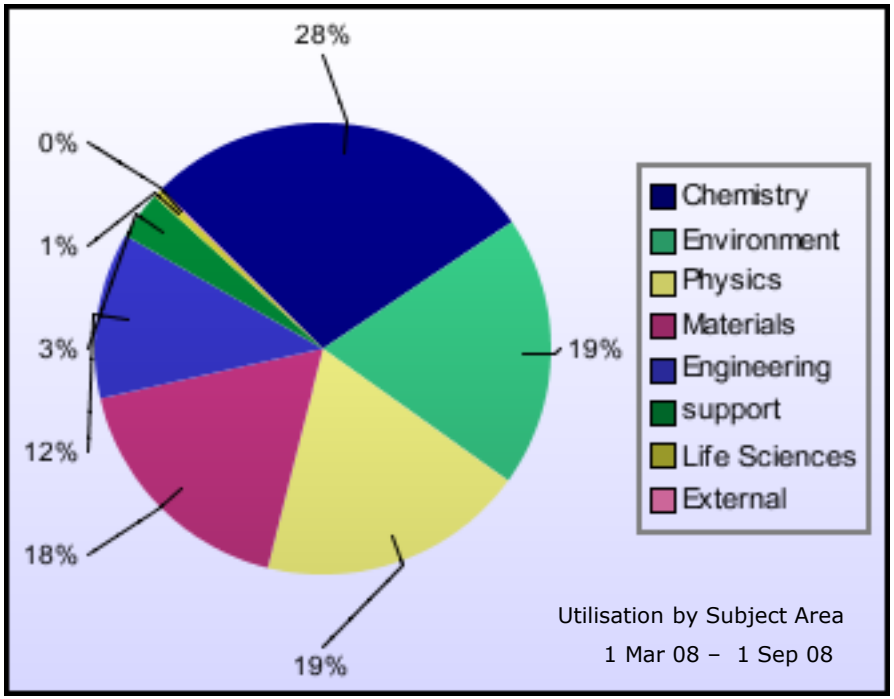
HECToR at the ACF

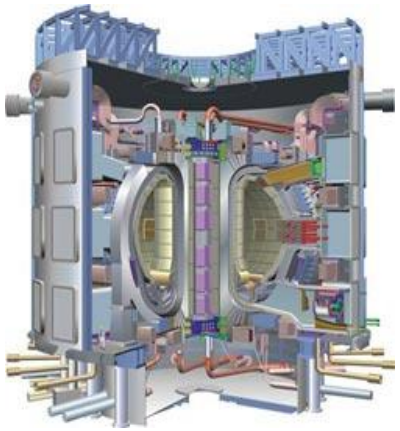
Current system:

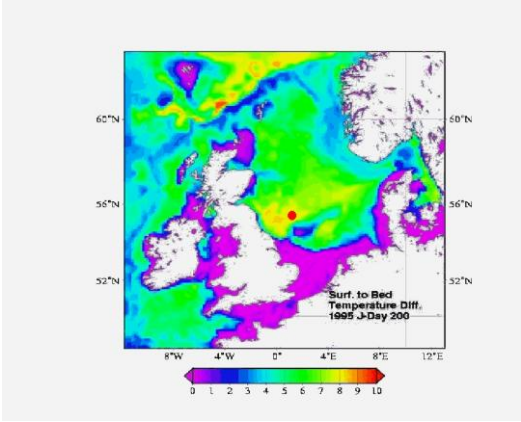
- Phase 2b
  - 20 cabinet Cray XT6
  - 44,544 cores
  - 59.4Tb memory
  - 360 Tflops
- Phase 2a
  - 33 cabinet Cray XT4
  - 12,288 cores
  - 24Tb memory
  - 1 cabinet Cray X2 with 112 vector processors
- Will soon get Gemini upgrade to XE6

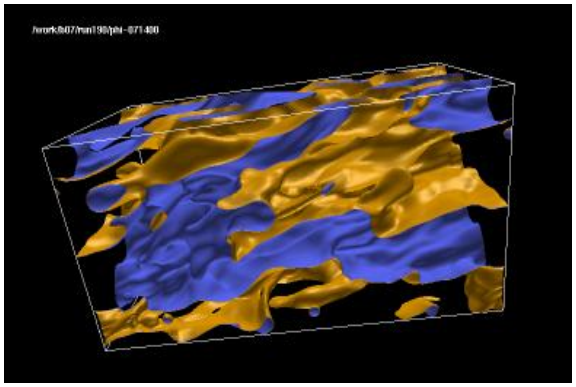
Utilisation by subject area

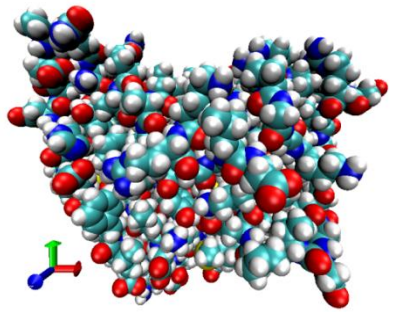
- Largest usage:
  - Chemistry
  - Environment
  - Physics
  - Materials











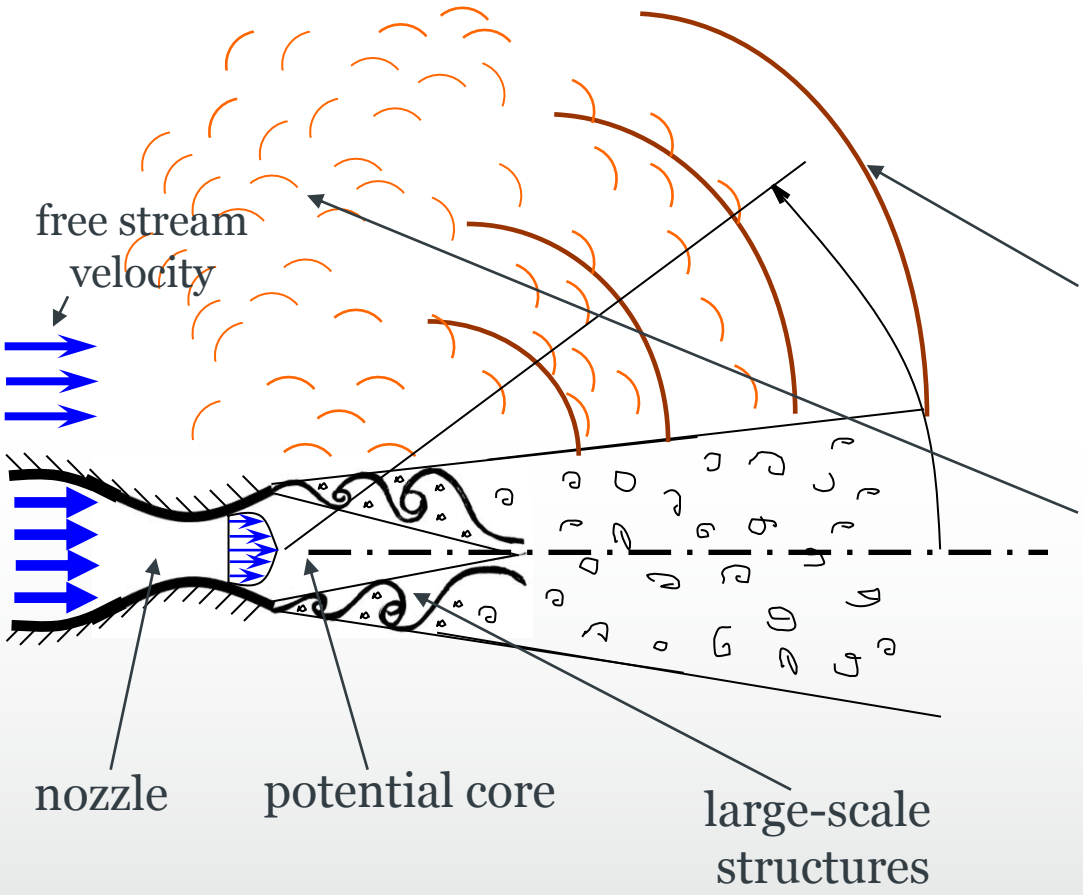
Cray Centre of Excellence

- As part of the HECToR service, the Cray Centre of Excellence provides in-depth support and direction for both current and future Cray HPC platforms through
  - advanced research into porting codes;
  - improving scalability of applications;
  - developing algorithms and system software tools; and
  - optimizing workload and I/O.
- Strong benefits to the HECToR research user community and amongst the other Cray Centers of Excellence around the world

Aeroacoustics of a jet engine

UNIVERSITY OF Southampton
School of Engineering Sciences

Dr Richard Sandberg



Radiated Sound:

Low-frequency sound
(highly directional)

High-frequency sound
(radiating in all directions)

Sound is radiated by several different physical mechanisms !

Numerical Method - HiPSTAR

UNIVERSITY OF Southampton
School of Engineering Sciences

(High-Performance Solver for Turbulence and Aeracoustics Research)

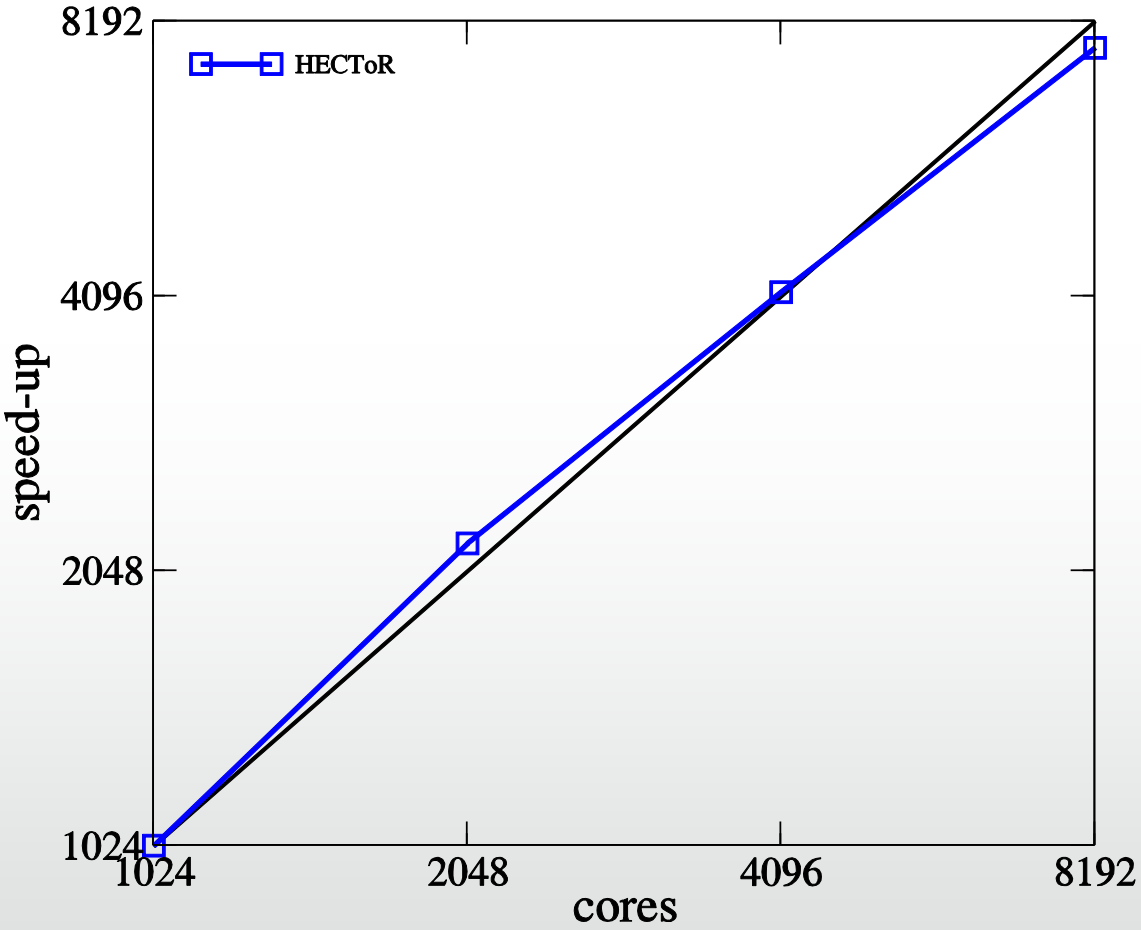
Compressible Navier-Stokes in curvilinear cylindrical coordinates

- 4th-order accurate finite difference scheme
  (standard or compact schemes using novel parallelisation technique)
- FFTW for discretisation of azimuthal direction
- Ultra low-storage 4^{th}-order R-K time-integration (Kennedy et. al, 2000)
- Skew-symmetric splitting of convective terms (Kennedy & Gruber, 2007)
- MPI-parallelisation via domain decomposition
- Nonreflecting zonal characteristic boundary condition
  → highly effective / free of coefficients (Sandberg & Sandham, 2006)

Numerical Method - HiPSTAR

UNIVERSITY OF Southampton
School of Engineering Sciences

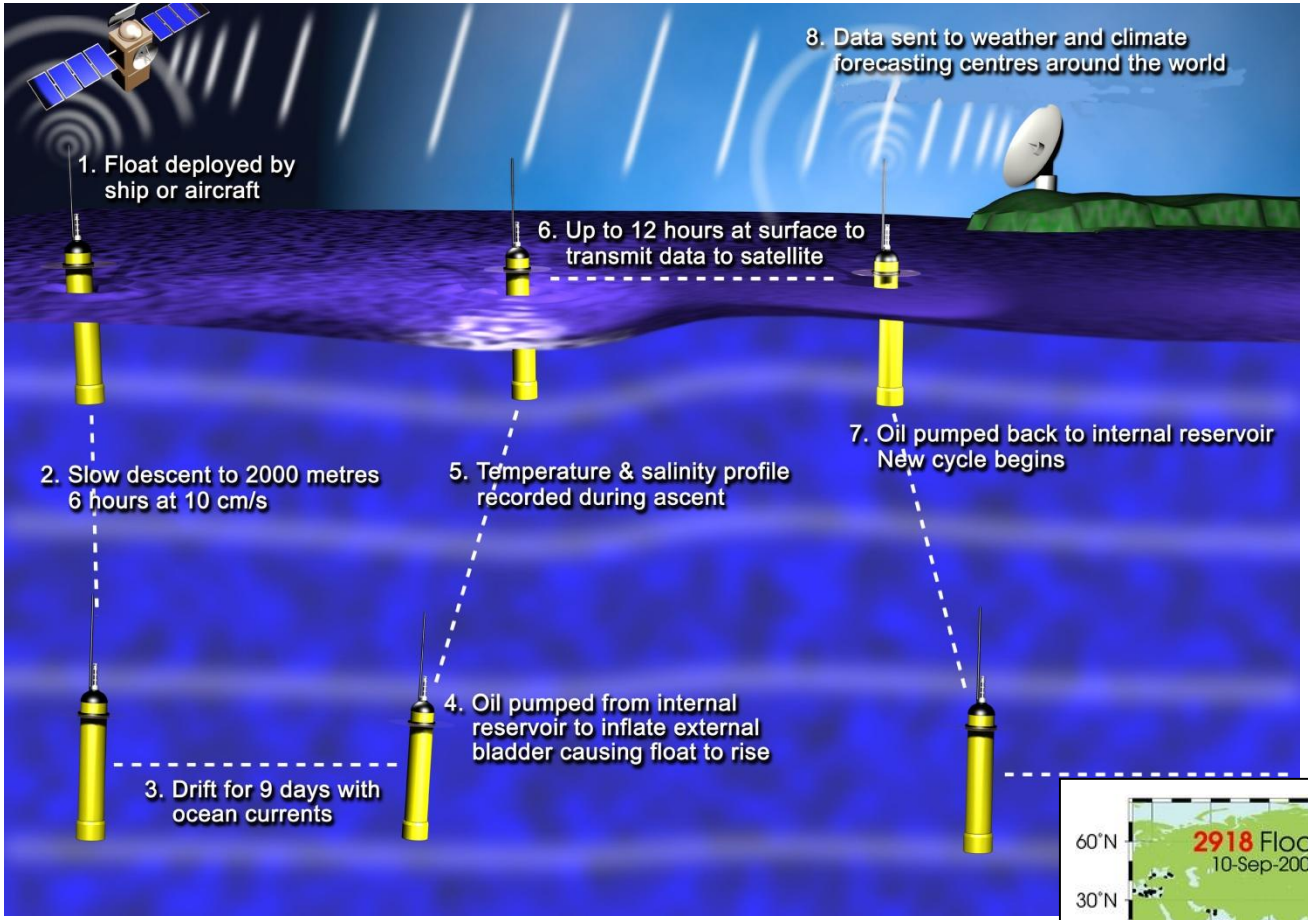
Production case with 3160 × 600 × 16 modes → ~70x10^6 points

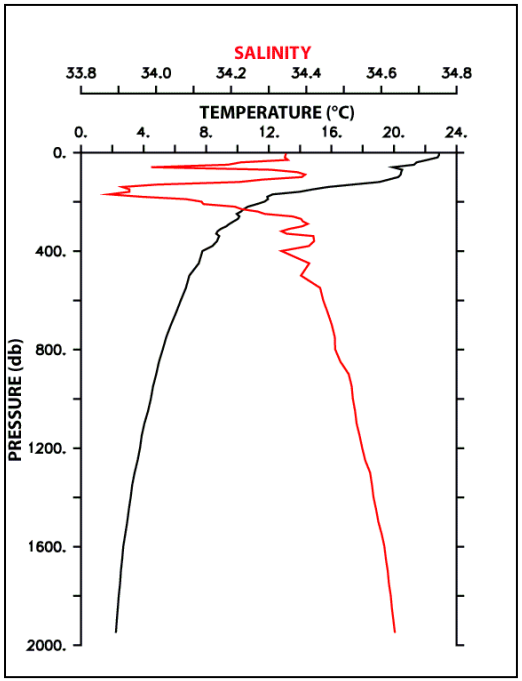


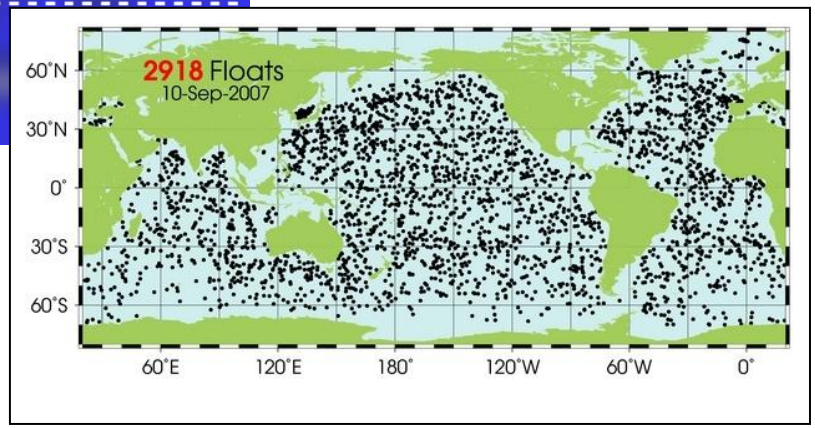
→ Excellent MPI scaling

Decadal Climate Predictions using HiGEM for the Argo Period

National Centre for Atmospheric Science
NATURAL ENVIRONMENT RESEARCH COUNCIL







Len Shaffrey
National Centre for Atmospheric Science
University of Reading

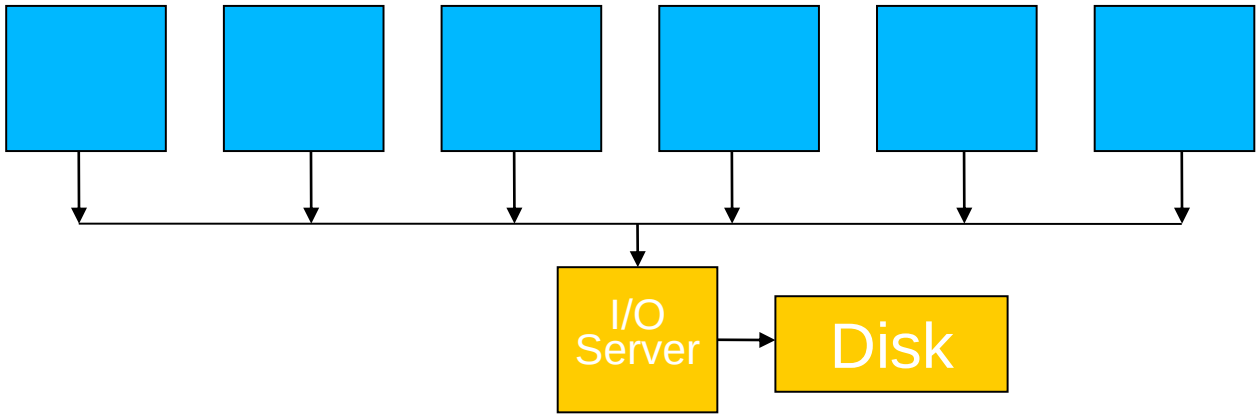
Technical Progress

National Centre for Atmospheric Science
NATURAL ENVIRONMENT RESEARCH COUNCIL

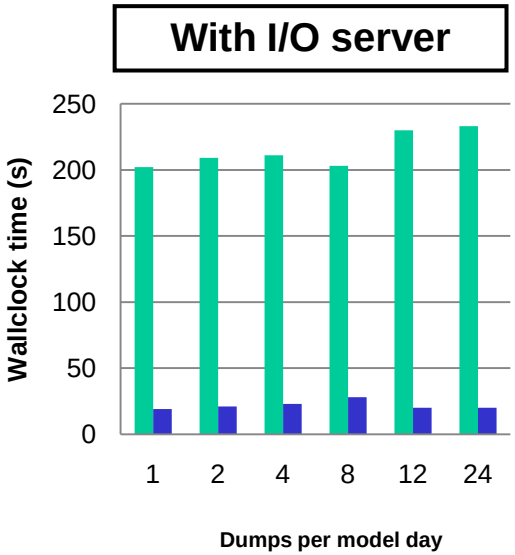
*HiGEM is based in the Met Office Unified Model. The **technical goal** of this project is to improve the I/O processes in the Unified Model.*

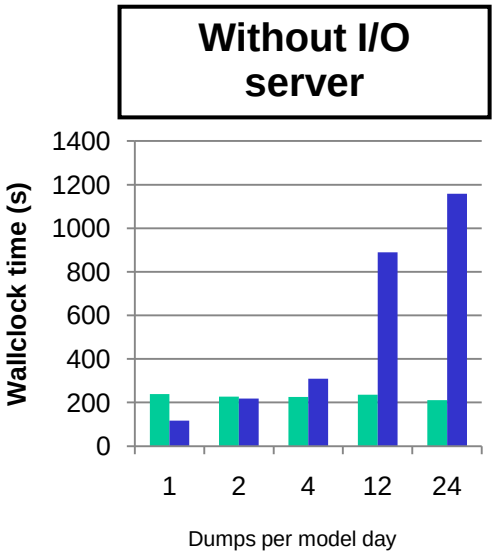
- *Implement a Cray developed I/O server*
- *Implement an ensemble framework for HiGEM*
- *Developments will be released at the end of the project to benefit Unified Model activities within the wider climate community*

The first task was to implement a Cray developed I/O server code. This assigns one (or more) processors as a dedicated I/O server. This asynchronous I/O should be more efficient



I/O server performance





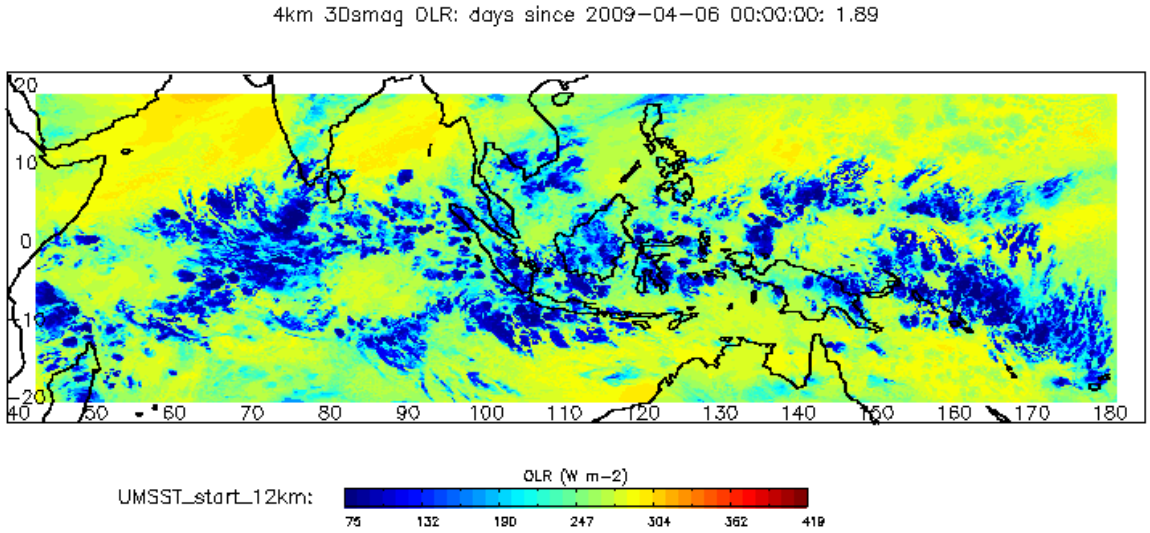
Sensitivity of the n216 Unified Model (run on 512 cores) to restart dump output frequency (dumps per day)

Light blue: time spent in compute routines

Dark blue: time spent in I/O routines

Previous performance problems overcome with buffering MPI calls

Implemented in Unified Model ensemble framework



Industry usage

- EPCC has worked with industry for nearly 20 years
- Majority of projects are bespoke software development projects with use of HPC systems
- EPCC Industry Hub provides focus for industry work
  - Relationships with ISVs
  - Focus on cycle sales and provision of access to codes
  - Brings all EPCC's industry activities together

- Support from Scottish Enterprise to enable new companies to make use of HPC simulations in their businesses through HPC Adopter Projects

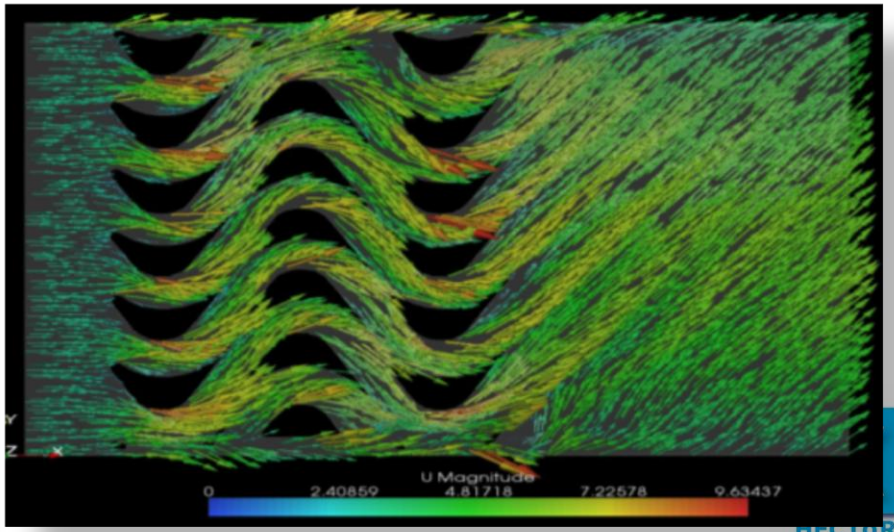
Deep Casing Tools – Turbocaser

- Deep Casing Tools is a privately owned SME in Aberdeen.
- Company focus is on innovative design combined with precision engineering that enable development and manufacture of the next generation of casing and completion tools for the oil and gas industry.

- Deep Casing Tools Turbocaser uses a motor powered by drilling-mud to ream oil wells prior to pipe installation.
- Important to understand and optimise the performance of the multi-stage motor.
- Drilling mud is a non-Newtonian fluid with Reynold's Numbers between 4,000 and 20,000 and densities typically between 1.1 and 1.4 g/cm 3.
- Very computationally expensive to performa multi-stage design studies.
- Ideal application for HPC: project modelled mud flow through various Turbocaser turbine designs using HECToR and OpenFOAM

Deep Casing Tools – Turbocaser simulation

- **Impact for company**
  - Validation of basic design
  - Better understanding of product behaviour
  - Optimisation of pressure drop versus torque across multistage turbine
  - Support for future product design and development
- **Impact for EPCC**
  - Demonstration of value of HPC to real world problem
  - Increased staff experience of CFD on HECToR
  - Extended use of OpenFOAM on complex problem
  - Potential for further use of HECToR eg. rotating mesh



Prospect – Wind & Wave Modelling

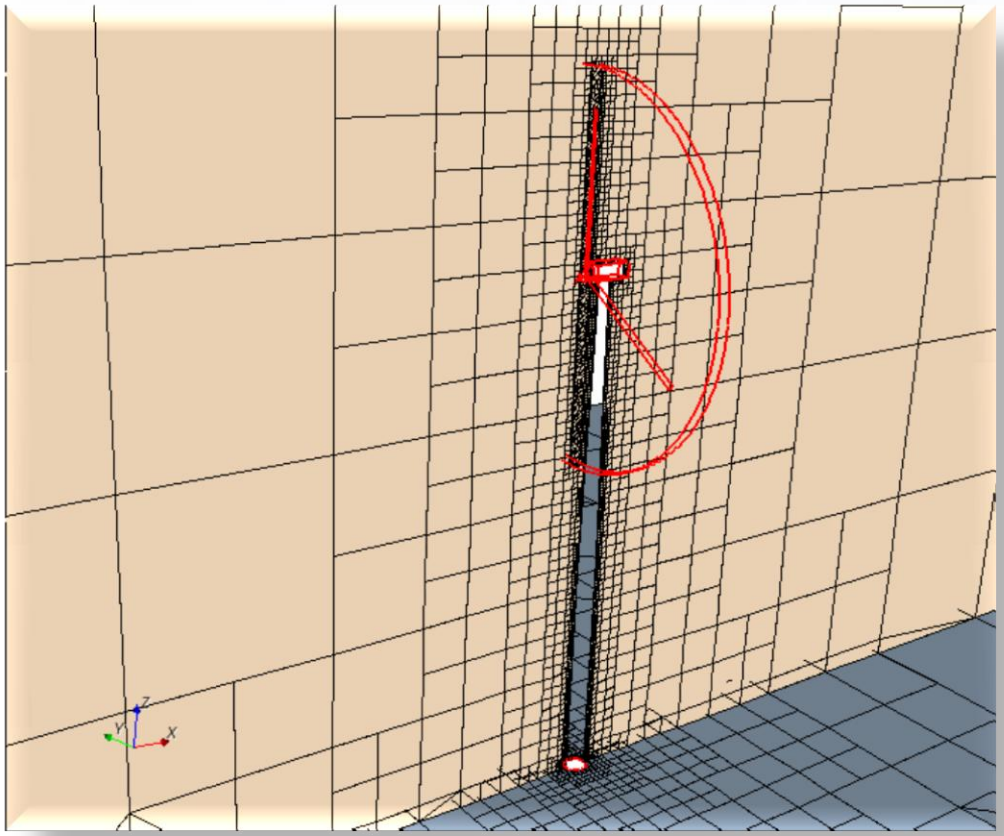
The Company:

Prospect is an engineering design and analysis provider to the world energy industries. Headquartered in Aberdeen, Prospect was founded by in 1999 and has grown rapidly since to become part of a 300 strong Group with operations spanning six continents

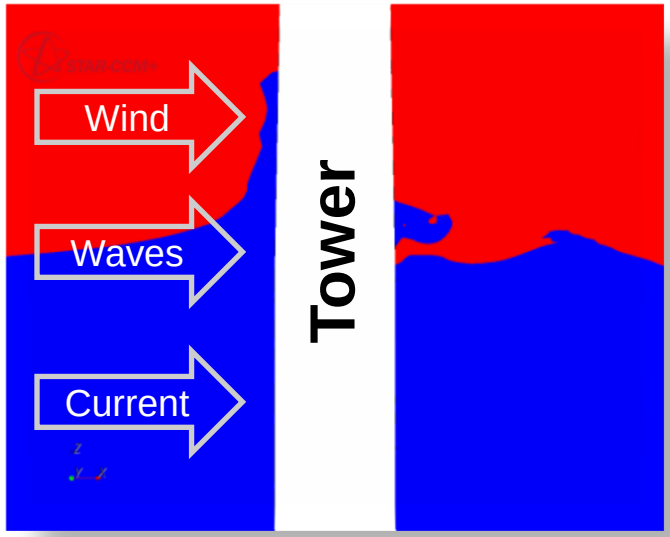
The Problem:

- Simulations exist of blades, turbine, wind on tower and waves on tower.
- Combining these simulations, using different software packages, is very difficult
- Massive computational resources required to keep all simulations sychronised
- **Ideal application for HPC**: EPCC asked to couple simulations and run result on HECToR

HPC solution: Coupled Simulation



- Create polyhedral / tetrahedral mesh to represent physical objects
- Simulate action of waves, ocean current and wind simultaneously
- Understand combined complex stresses on structure



Tools:

Simulia-Abaqus Finite Element Analysis
StarCCM Computational Fluid Dynamics

Final comments

- We are at a very exciting moment in supercomputing
- Many challenges at the hardware and software level face us a systems get bigger, more energy hungry and more difficult to program
- But ... modelling and simulation brings enormous scientific and economic benefits to those who invest in it

Enjoy your Cray!

Thank you