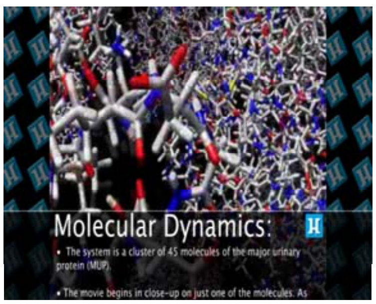
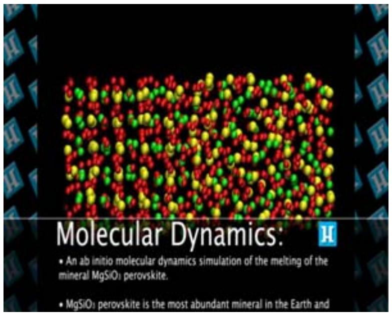
HECToR Launch Movie Transcript

About HECToR
o HECToR: a £113m service that will run for six years .
o A world-class service for UK-based academic research.
o Capable of 63 million million calculations a second.
o Represents the equivalent of approximately 12,000 desktop systems.
o An initial theoretical peak capability of 63 Tflop/s.

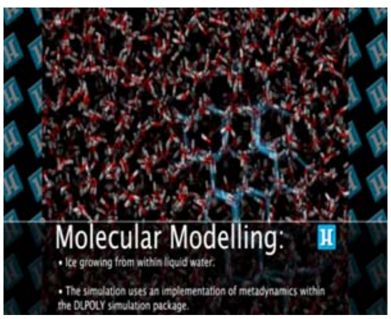


Molecular Dynamics (1)
o The system is a cluster of 45 molecules of the major urinary protein (MUP).
o The movie begins in close-up on just one of the molecules. As the dynamics progresses, it zooms out to show the full size of the simulated system.
o At just under a million atoms, this is a very big simulation by current standards.
o It was designed to show that HECToR allows simulations that would exceed the capabilities of smaller compute systems.



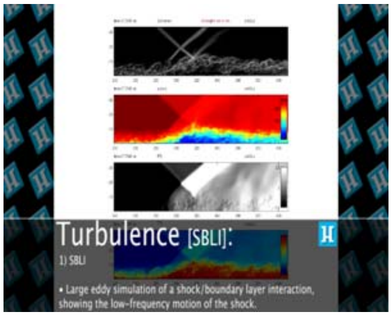
Molecular Dynamics (2)

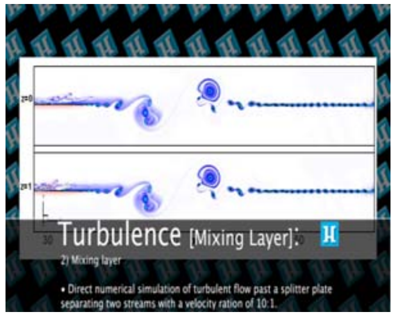
o An ab initio molecular dynamics simulation of the melting of the mineral MgSiO3 perovskite.
o MgSiO3 perovskite is the most abundant mineral in the Earth and exists at depths from 670 km to 2970 km in the Earth's mantle.
o This simulation is run at a temperature of 5700 K and a pressure of 60 GPa (about 1800 km depth) and shows the solid (left hand side) gradually melting.
o A similar simulation at a slightly lower temperature of 5500 K does not melt.
o This shows that the melting temperature of this mineral is about 5600 K at this pressure.



Molecular Modelling

o Ice growing from within liquid water.
o The simulation uses an implementation of metadynamics within the DLPOLY simulation package.
o HECToR has allowed the simulation of sufficiently large systems that the growth of the ice nucleus is not hampered by simulation boundary effects.
o Hydrogen bonds that have been identified as belonging to ice clusters are highlighted.





Turbulence

1) SBLI

o Large eddy simulation of a shock/boundary layer interaction, showing the low-frequency motion of the shock.

o Shock-induced boundary layer separation can occur in a range of external and internal flow problems in aerospace, such as supersonic intakes and turbomachinery, and significantly affects heat and unsteady pressure loads.

o Instantaneous contours of the density gradient (pseudo-Schlieren), the streamwise velocity component, pressure and temperature (top to bottom) are shown.

o The Reynolds number based on the displacement thickness of the boundary layer at impingment is 20000, the pressure ration of the shock is 2.5 and the Mach number is M=2.3.

o The simulation was conducted using 1 million grid points distributed over 1024 processor cores on HECToR.

2) Mixing layer

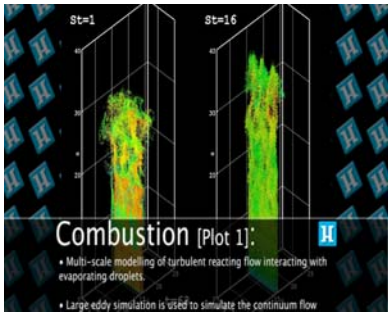
o Direct numerical simulation of turbulent flow past a splitter plate separating two streams with a velocity ration of 10:1.

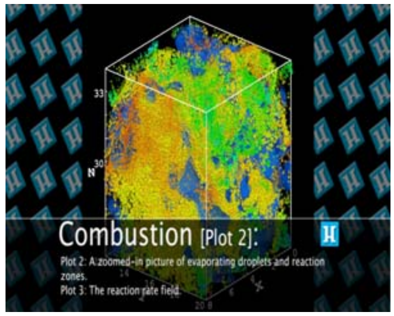
o This is a canonical example for mixing layers encountered in many applications, for example jets flows. Understanding the generation and evolution of large coherent turbulent structures is relevant for the prediction of aerodynamic performance and the noise generation.

o Instantaneous contours of the spanwise vorticity component are shown at planes with different spanwise positions. The Reynolds number based on the displacement thickness of the upper boundary layer at separation is approximately 2300 and the Mach number is M=0.6

o The case was performed using nearly 500 million grid points distributed over 2048 processor cores on HECToR.

o Work created as part of the EPSRC UK Turbulence Consortium (EP/D044073/1)





Combustion
o Multi-scale modelling of turbulent reacting flow interacting with evaporating droplets.
o Large eddy simulation is used to simulate the continuum flow and temperature fields coupled with a Lagrangian formulation for discrete droplet dynamics (Xia and Luo, 2007).
Plot 1: Evaporating droplet dynamics at two Stokes numbers with colours representing temperature levels.
Plot 2: A zoomed-in picture of evaporating droplets and reaction zones.
Plot 3: The reaction rate field.
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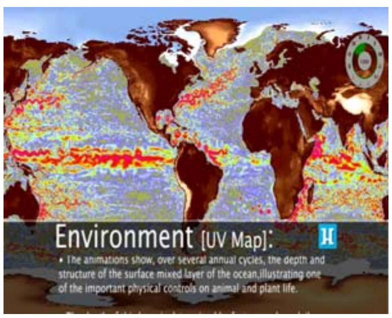

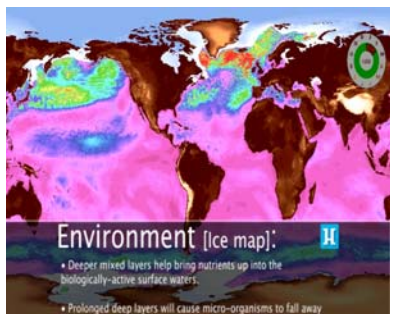

Environment
o The animations show, over several annual cycles, the depth and structure of the surface mixed layer of the ocean, illustrating one of the important physical controls on animal and plant life.
o The depth of this layer is determined by factors such as daily and seasonal heating cycles, energy input from surface winds and local stratification of the surface waters.
o Deeper mixed layers help bring nutrients up into the biologically-active surface waters.
o Prolonged deep layers will cause micro-organisms to fall away from the light-penetrated layers and stop productivity.
o The ocean's biology is therefore critically sensitive to small spatial and rapid temporal variations in the mixed layer depth (These animations were not created using HECToR).