The Hartree Centre

An International Centre for Computational Science and Engineering

Positioning the UK to take a World Leading Role

Science & Technology Facilities Council

Science & Technology
Facilities Council

- *Simulation and modelling can play a key role in all areas of science*

- *UK has world class expertise in Computational Science and Engineering (CSE)*

- *Fragmented – needs a national focus and Centre of Excellence for critical mass*
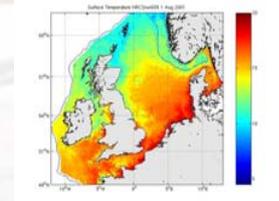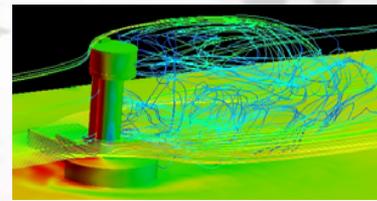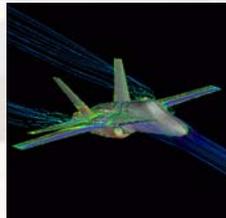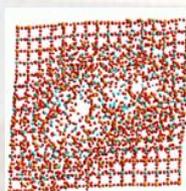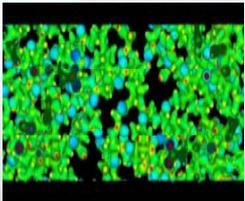
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The Background II

- *Campus development at Daresbury and Harwell – partnering academia, industry & STFC*

- *CSED supports a world class activity in applications and HPC*

- *STFC investment in Gateway*

   Technology Centres (GTCs)

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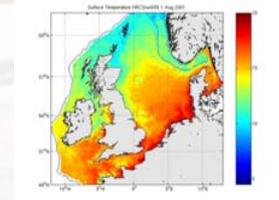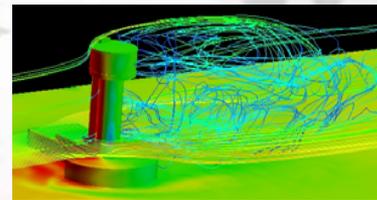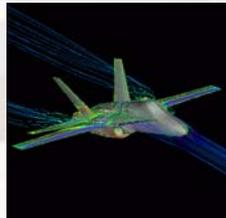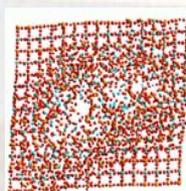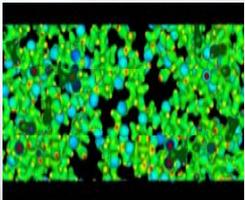
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GTCs and Science Directions

	Hartree Centre	Facilities	Advanced Materials	Design, Engineering	Detectors
Biosciences and Health Care					
Energy Technology					
Climate Change and Environment					
Global Threats to Security					
Nanoscience and Nanotechnology					
Digital Economy					

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Hartree Centre Mission Statement

"The Hartree Centre at the Daresbury Science and Innovation Campus will be a new kind of computational sciences institute for the UK.

It will bring together academic, government and industry communities and focus on multi-disciplinary, multi-scale, efficient and effective computation.

The goal is to provide a step-change in modelling capabilities for strategic themes including energy, life sciences, the environment and materials"

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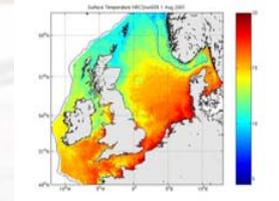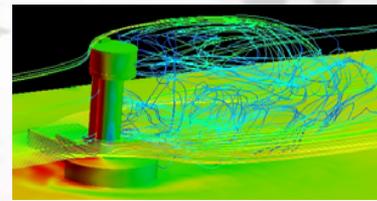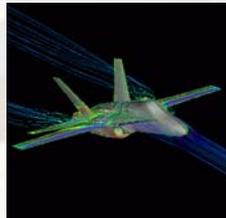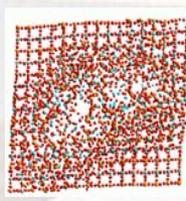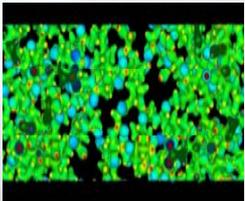
Delivering grand challenge solutions with world-leading partners

- *Energy*
- *Environment*
- *Functional Materials*
- *Life Sciences*

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The Challenge - Integrative Science

Science & Technology Facilities Council

Continuum
FE, CFD,…

μ-Fluidics

Mesoscale
DPD, CG, LBM, Kinetic MC

NanoScale
Classical MD

Quantum
DFT, CCSD(T)

| | s | ms | μs | ns | fs |

Atoms : | 1 | 10^3 | 10^8 | 10^{12} | 10^{21} | 10^{24} | m

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The Challenge - Integrative Science

s —

ms —

μs —

ns —

fs —

Gas Flows

Kinetics of surface species populations

Diffusion, aggregation

Catalytic Chemistry

Example - Fuel Cell Modelling

Å   nm   μm   mm   m

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Integrating Capabilities

Step change solution!

International Links

Compute Resources

Code Development

Science Grand Challenge Projects

Science Expertise

Software Engineering

Training

Collaborative Environment
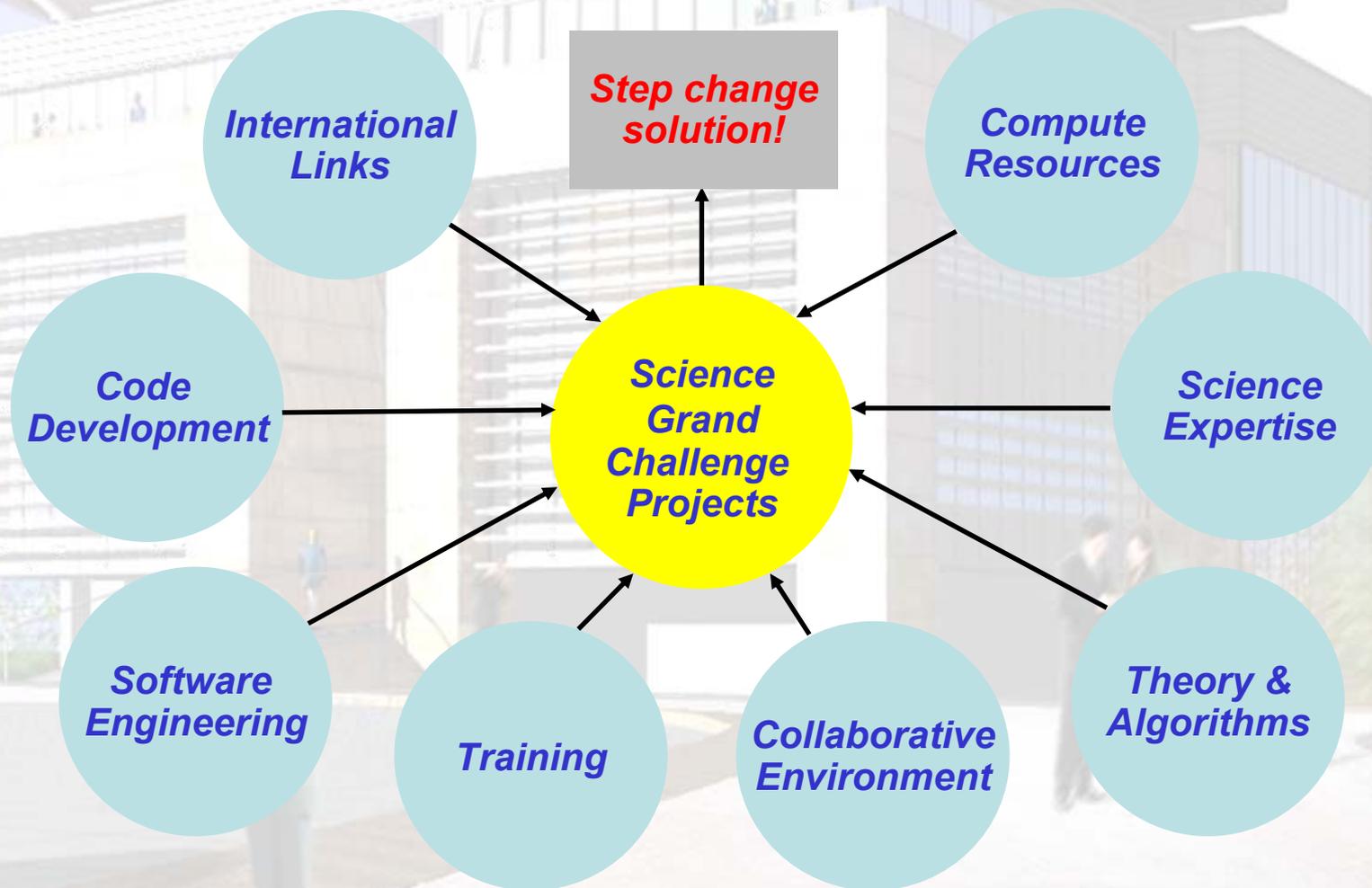
Theory & Algorithms

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Grand Challenge Projects I

Projects will:

- *Bring together leading CSE groups*
- *Develop next generation theory, algorithms and codes*
- *Require significant computational resources*
- *Be internationally leading*
- *Generate long-term collaborations*
- *Be aligned with Government and STFC science strategy*

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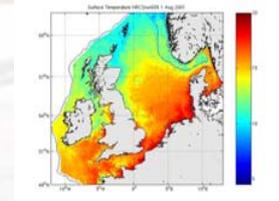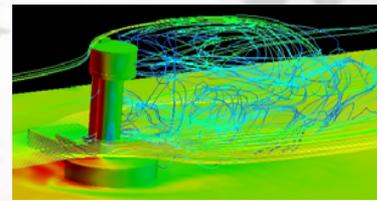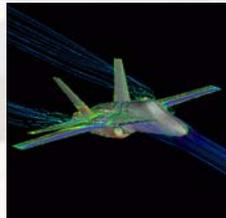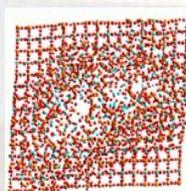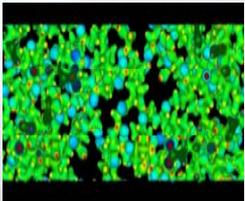
- *Predictive combustion*
- *Whole device modelling of fuel cells*
- *Hydrogen storage*
- *Photovoltaics*
- *Biofuel processes*
- *Nuclear fuels and waste containment*
- *HiPER – fast ignition route to fusion*

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Environment
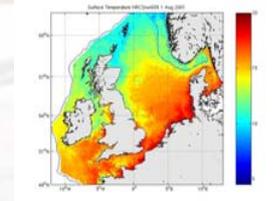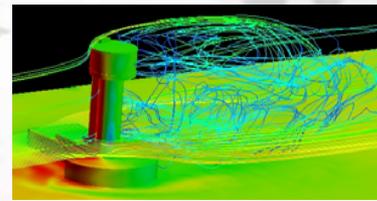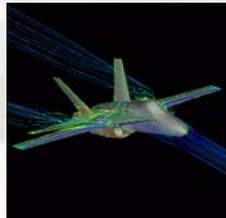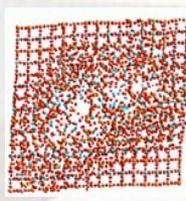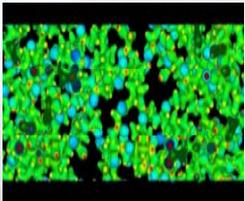
- *High-resolution long-term climate ensembles*
- *Quantifying climate variability and probability of extreme events*
- *Global coastal & shelf sea modelling*
- *Whole basin arctic simulation*

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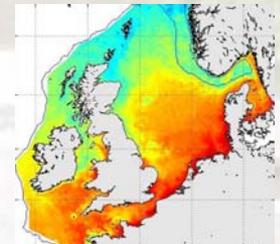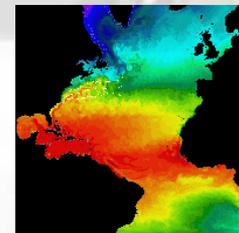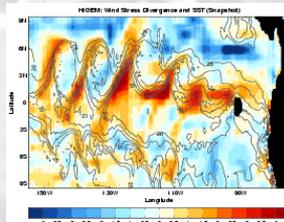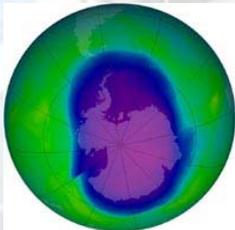
Functional Materials

- *Predicting phase diagrams of complex materials*
- *Understanding catalysts*
- *Characterisation of nanostructures*
- *Developing new spin devices*
- *Molecular electronics materials*
- *Superconducting materials*

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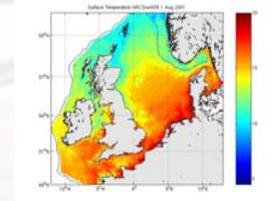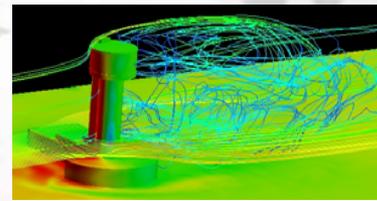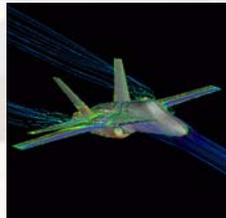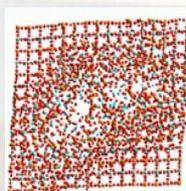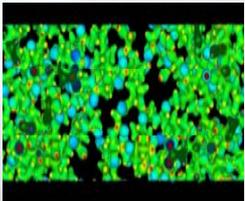
- ***Whole Cell Modelling – SimCell***
  - *Development of 'continuum' cell models for use in SimOrg*
- ***Whole Organism Modelling – SimOrg***
 - *Development of models of tissues, organs, systems and organisms*
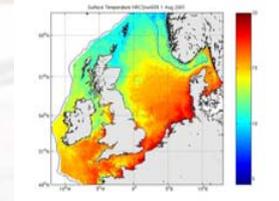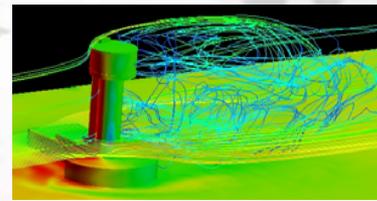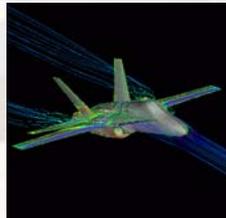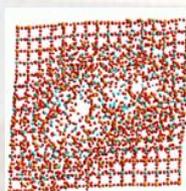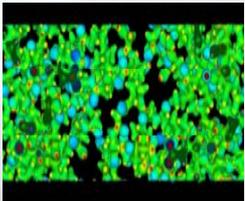
Grand Challenge Projects II

- *'Front Cover of Nature' quality and impact*
- *Deliver step change in modelling*
- *Lead to significant KE opportunities*
- *Small number of projects (3-6) at any time*

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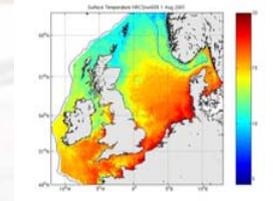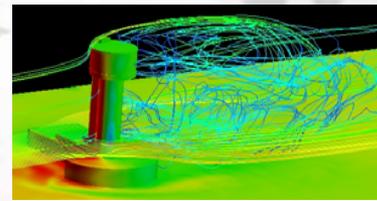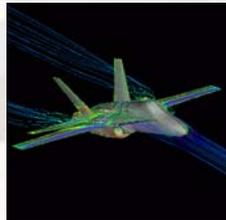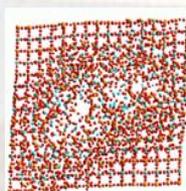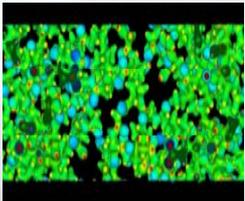
# Technology Challenges: Realising the Potential

- *Scalable algorithms*

- *Management of memory hierarchy*

- *Fault tolerant computing*

- *Data management and visualization*

- *Performance analysis*

- *Software engineering*

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Delivering
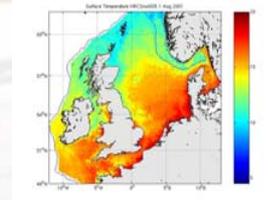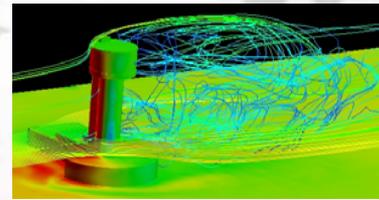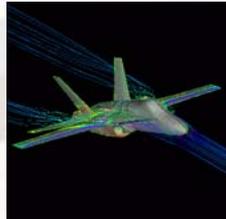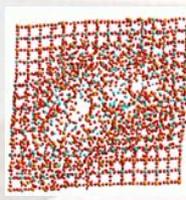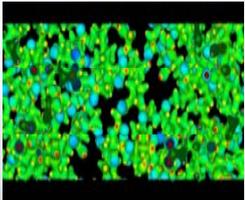
- *Major targeted scientific advances*
- *World-leading software developments*
- *A purpose built collaborative CSE environment*
- *Education and training*
- *Step change in knowledge exchange through the DL Campus*

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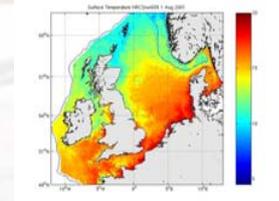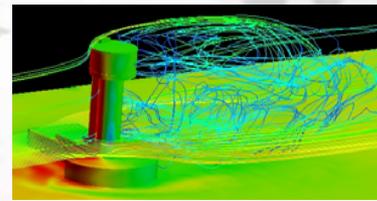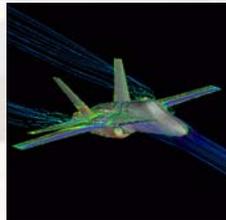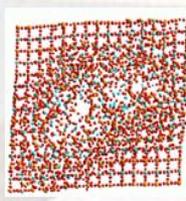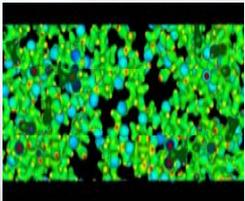
A REAL not a Virtual Institute

- *Located at Daresbury Science and Innovation Campus (DSIC)*
 - *Maximise Knowledge Exchange*
  - *Maximise Economic Impact*

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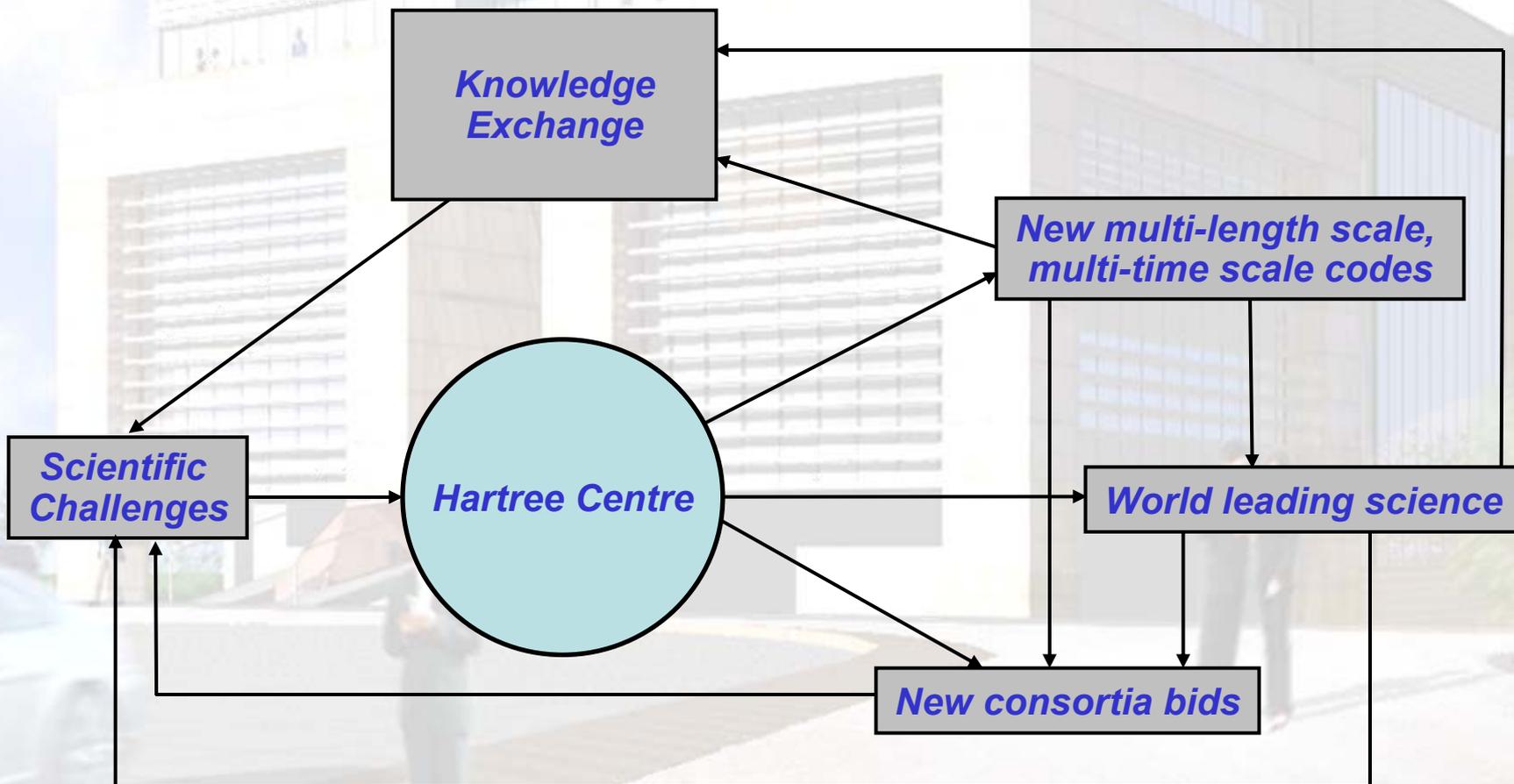
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- *Science-led*

- *Industrially and commercially relevant*
  - *Skills - Training, Consultancy*
 - *Facilities - Computer systems, Machine room, Training suite*

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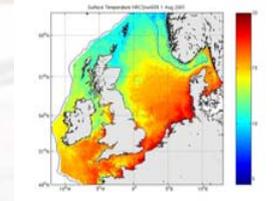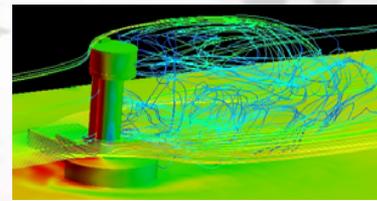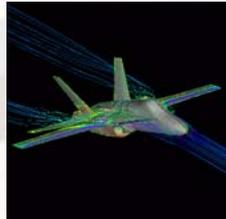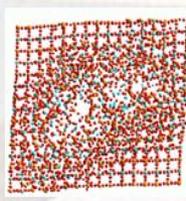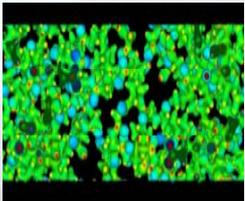
- *Solutions*

  Code parallelisation and optimisation

  New product design & service development

- *Intellectual Property*

  Sharing

  Generation

  Exploitation

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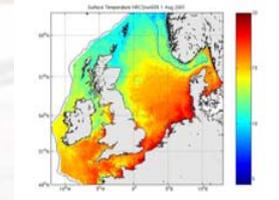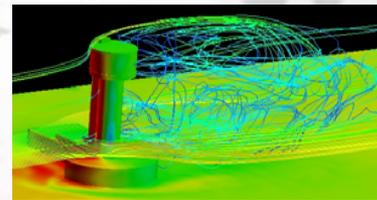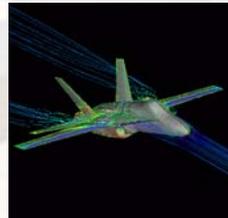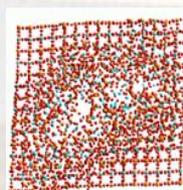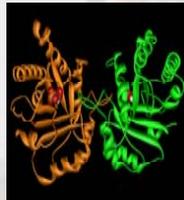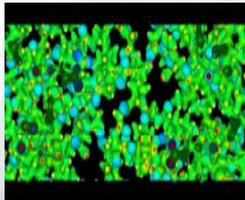
Infrastructure

- *A CSE centre with 100+ staff*

- *Attractive working environment*

- *Large scale compute resource*

- *Recurrent circa £16 Million pa*

- *Capital costs circa £50 Million – bid to LFCF*
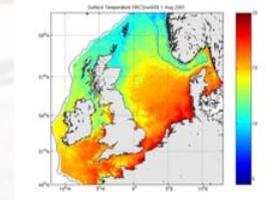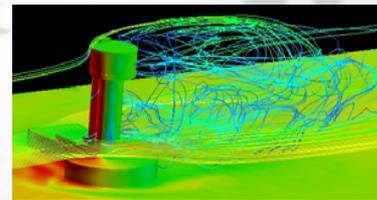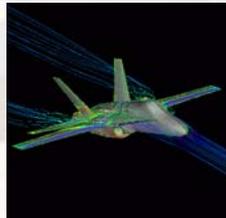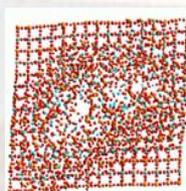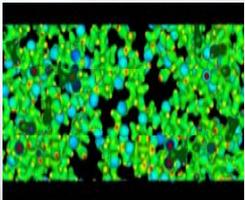
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# *Working with the Universities & Facilities*

Partner with Universities to grow

- *Joint appointment of staff*

- *Secondment and sabbaticals*

- *Collaboration with facilities*

- *Joint hardware procurement*
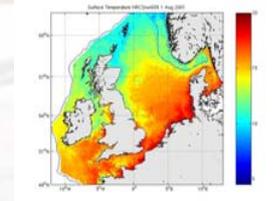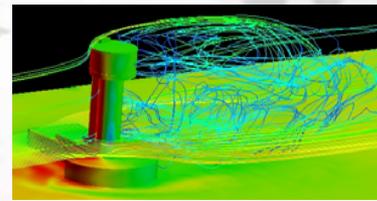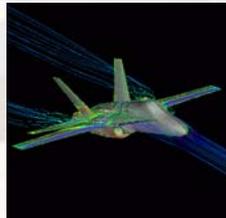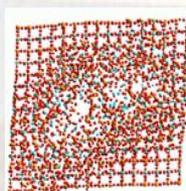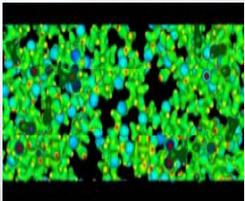
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Working with the Universities & Facilities

- **Skills**
  - Access to broad and deep skills of CSED staff
  - Develop code for new/ existing CSE and HPC applications
  - Porting and optimisation, procurement support, hosting of kit, …
 - Access to STFC technology

- **Joint Funding Opportunities**
  - Collaborators, joint applicants for funding, RCs, TSB, Europe, NWDA, ..
  - Sabbaticals and also shorter term placements related to specific objectives
  - Access to national/ international collaborators and projects

- **Training**
  - Joint supervisors, as teachers, examiners …
  - Development of computational science courses
  - Training programmes

- **Knowledge Exchange**
  - CSE/ HPC marketing activities – facilities, codes and solutions
  - Environment for HPC/ CSE spin-out activities
 - Development of new industrial Consortia

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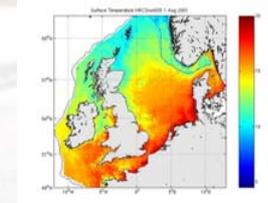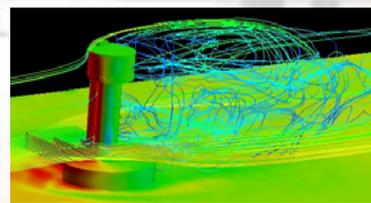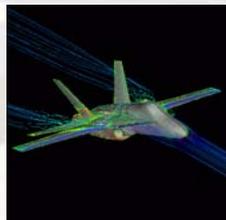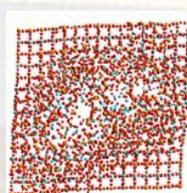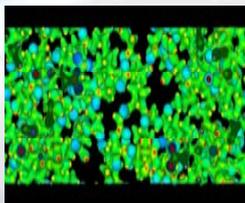
- **The Hartree Centre will provide training in Theory, CSE and HPC:**
  - *Postgraduate students in liaison with DTCs*
  - *Industrial scientists to exploit CSE and HPC*
  - *STFC facilities scientists*
- **The Centre will host international training schools and conferences**
- **The Centre will promote awareness of CSE through seminars for schools and the public**

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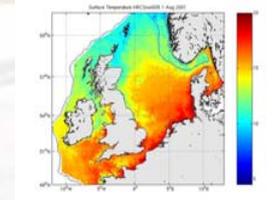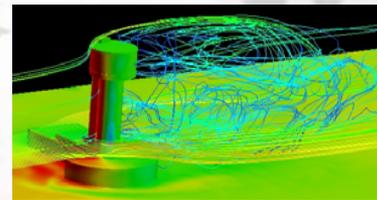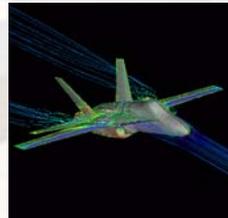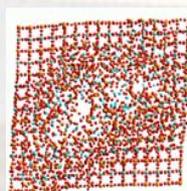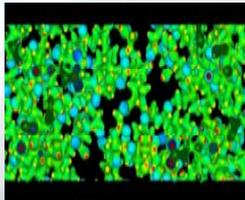
## *International aspects are central to the vision. The Centre plans:*

- *to attract the best computational researchers in the world to the UK as visitors*

- *to forge active collaborative partnerships with key overseas institutions*

- *to participate in and lead relevant international initiatives and networks*

- *to host a series of international workshops and conferences;*

- *to use all these activities to leverage international business development and knowledge exchange.*
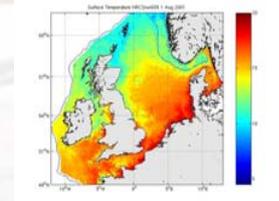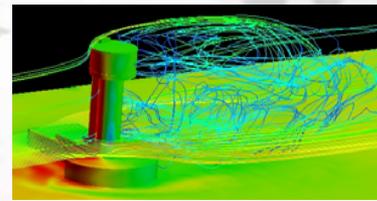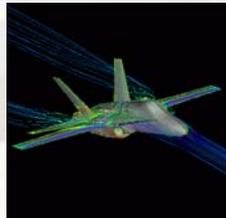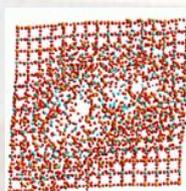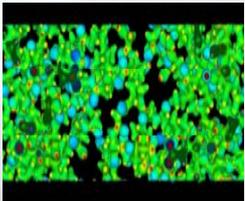
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On 14th July DIUS announced £397 million funding for world leading research facilities

"The approved projects include:
*£50 million for a new computational sciences centre at the Daresbury Science and Innovation Campus"*

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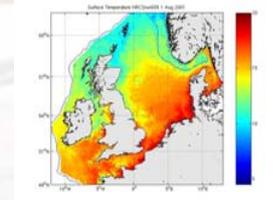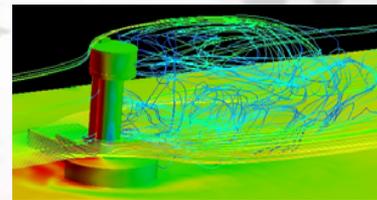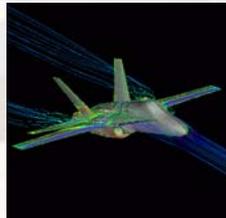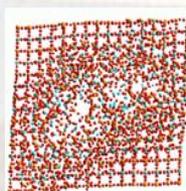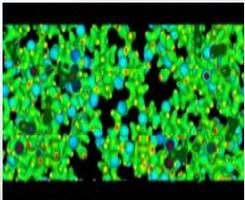
*http://nds.coi.gov.uk/Content/Detail.asp?ReleaseID=373716&NewsAreaID=2*

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- ***Build Hartree Centre – operational 2 years from final approval***
- ***Bid to STFC for core funding for:***
  Code development grants line
  Recurrent costs for Hartree Centre
- ***Complemented by bids for specific projects:***
  8 workshops covering key science themes focussing on petascale and exa-scale applications
- ***Academic partners***
  Regional and national centres of expertise
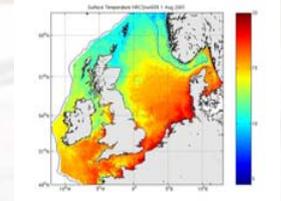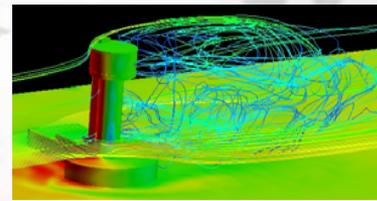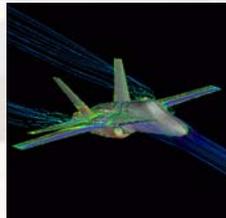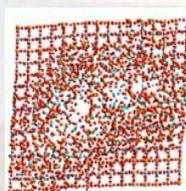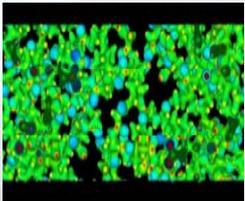
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KE consultations:

Virtual Research in Engineering Centre (NWAA, BAE systems, Liverpool, ..)

Knowledge Centre for Materials Chemistry (Unilever, AZ, Fujifilm, ICI, Solvay, Chemistry Innovation, ..)

*Centre for Earth Systems Intelligence (Lloyds, IBM, ..) - under development*

Nano-packaging for veterinary applications - under development

Blue chip vendor discussions (IBM, Cray, Intel, Microsoft, …)

System Integrators (OCF, Clustervision, ..)

Commercial software providers (Accelrys, Ansys/ Fluent, AspenTech,..)

*Industrial end-users (as above, Waters, Thales, AZ, BP Chemicals, DSIC, ..)*

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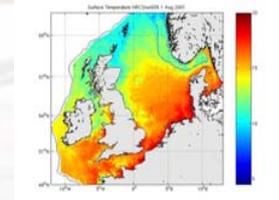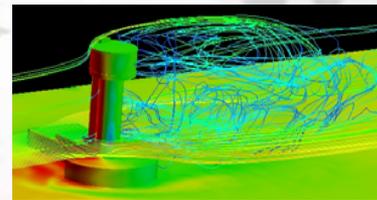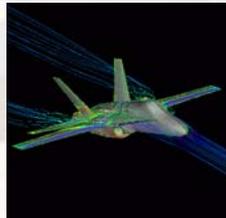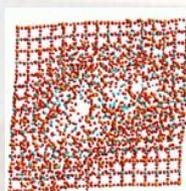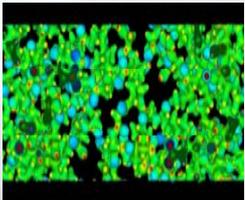
Timetable

Formation of project teams	*April 2008*
Science workshops	*July 2008*
Outline business case	*July 2008*
Detailed business case	*October 2008*
Public launch of first GTCs	*December 2008*
Review of progress	*End 2009*
Operational Hartree Centre	*2010*
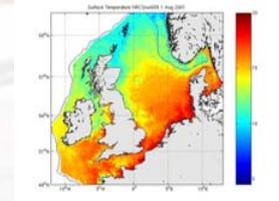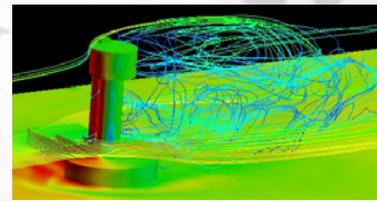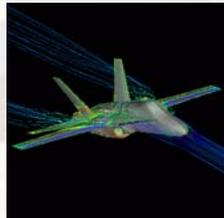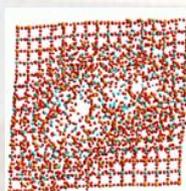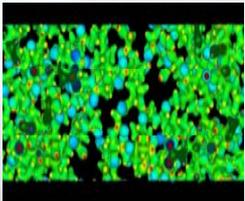
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The Hartree Centre

The Hartree Centre Will Deliver a World Class UK Research Institute Capable of Partnering with Major US and International Labs

A Step Change in the UK's CSE and KE Capabilities

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