

The Collaborative Computational Projects (CCPs)

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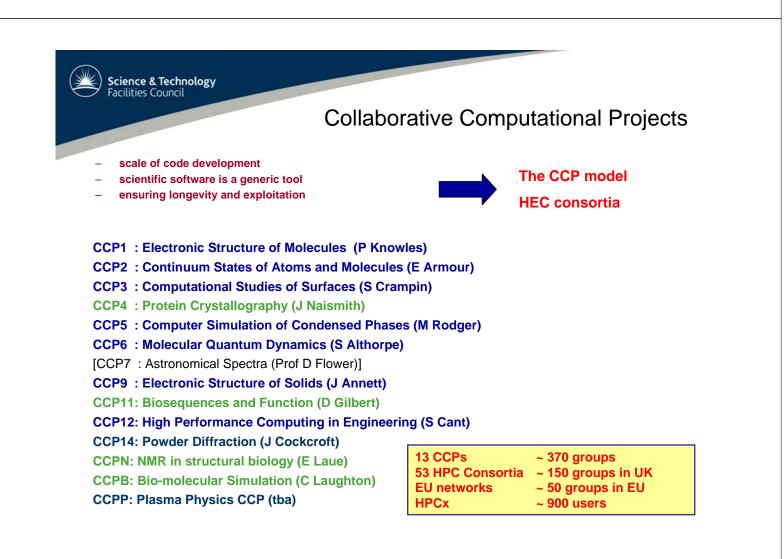
- What are the CCP's?
- Science an Technology Facilities Council
- Computational Science and Engineering @ STFC
- The Hartree Centre
- Conclusions



UK Code Development

- Development and distribution of high quality software does not fit easily into the 'three year' academic grant cycle
- Need to maximise return on investment in code development
- The CCP model longevity of codes

http://www.ccp.ac.uk





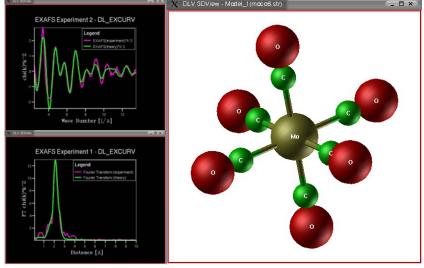
Collaborative Computational Projects

- Provide a topical software infrastructure from the desk-top to the most powerful supercomputing facilities
 - advancing CSE and 'theory of the experiment'
 - Implement "flagship" code development projects
 - Maintain and distribute code libraries
 - Organise training in the use of codes
 - Hold meetings and workshops
 - Overseas researchers for lecture tours and collaborative visits
 - Issue regular newsletters
- Of order 500 papers per year ~ 10% "hot news" category
- Overseas links MOLSIMU, CECAM, psi-K, LightNet,...
- Overseen by CCP Steering Panel, chaired by Prof P Coveney includes CCP Chairs, Director of CECAM and international members

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LighTneT and Facilities

A major new collaboration on theoretical support for light source facilities has been established and funded by the EU at the level of 1 million Euro's. This represents an International outreach of CCP3's activities



Move towards internationalisation of the CCP's European collaboration funded by EU – Japan?

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Scientific Highlights ...

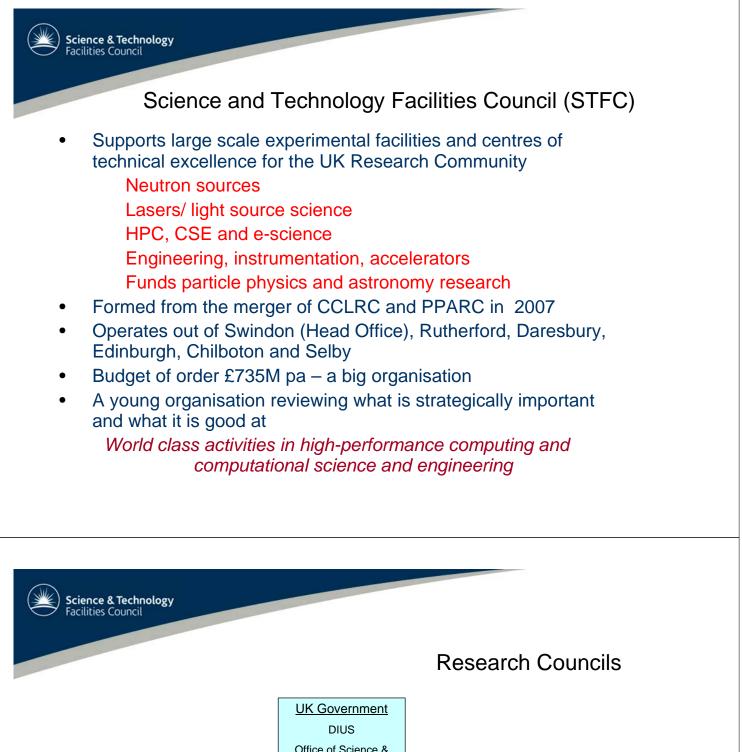
- Journal of Materials Chemistry <u>16</u> no. 20 (May 2006) issue devoted to HPC in materials chemistry (esp. use of HPCx); CCP1, CCP3, Mat Sci Consortium
- Phys. Stat. Sol.(b) <u>243</u> no. 11 (Sept 2006) issue featuring scientific highlights of the Psi-k Network (the European network on the electronic structure of condensed matter coordinated by our Band Theory Group); CCP9, UKCP Consortium
- Molecular Simulation <u>32</u> no. 12-13 (Oct, Nov 2006) special issue on applications of the DL_POLY MD program written & developed by Bill Smith (the 2nd special edition of Mol Sim on DL_POLY - the 1st was about 5 years ago); CCP5
- Acta Crystallographica Section D <u>63</u> part 1 (Jan 2007)
 proceedings of the CCP4 Study Weekend on protein crystallography. CCP4
- The Aeronautical Journal, Volume 111, Number 1117 (March 2007), UK Applied Aerodynamics Consortium, Special Edition. CCP12

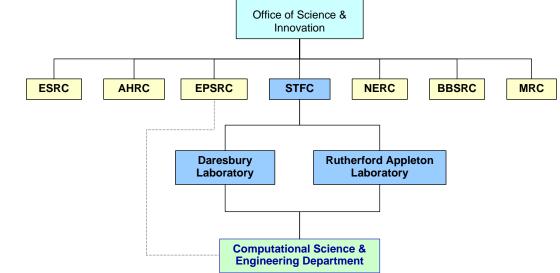


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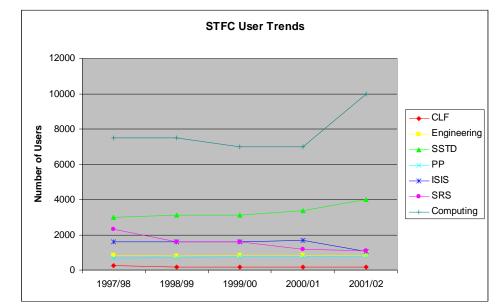
Long Term Support for CCP's

- Long term support for development, distribution, documentation and training has been key to the success of the CCP's
- Support provided (for many of the CCP's) by staff effort within the Computational Science and Engineering Department at STFC Daresbury (Rutherford) Laboratory
- Funded by 'Service Level Agreement' (SLA) with the Engineering and Physical Sciences Research Council (EPSRC)









How Important is the Computational Science Community to STFC?

Figures taken from STFC Annual Reports – more recent Reports do not give user numbers.

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> Mission: "Ensuring that UK researchers benefit from the best computational methods and techniques"

Computational Science and Engineering Department

Major funded activities

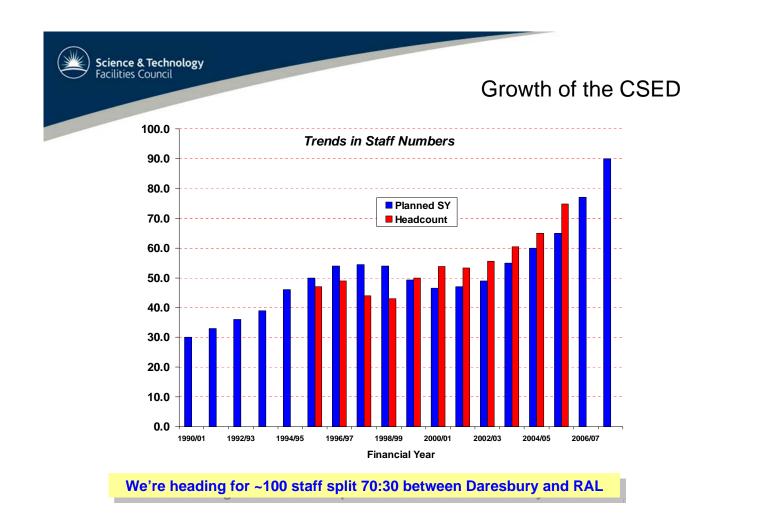
– Research,

Vision: "To be the focus for the development, application and support of a vibrant world-leading UK research programme in CSE"

- Applications development and support CCPs and HEC Consortia
- Compute and data facilities and services HPCx
- 80 staff £7M pa turnover
- International collaborations

All underpinned by an R&D and support programme in technical computing

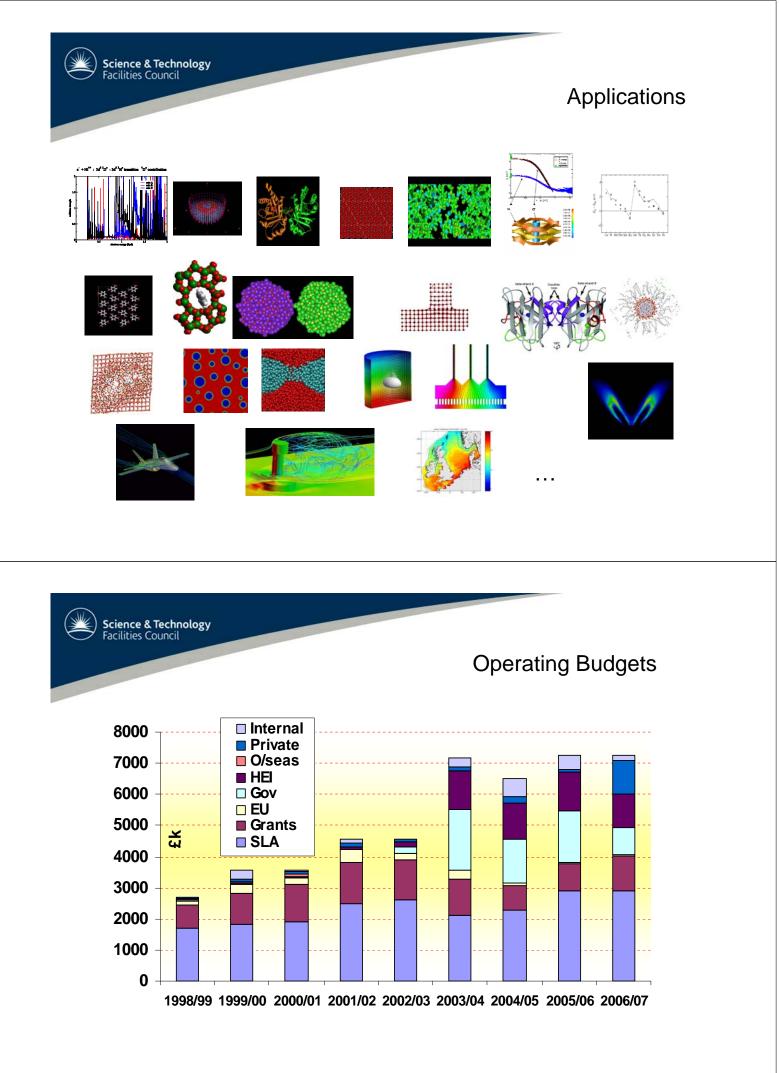
- Major science themes and capabilities
 - Atomic and Molecular Physics
 - Bioscience gone from zero to a 20% activity in 5 years
 - Condensed matter physics and materials
 - Computational chemistry quantum, classical and coupled simulations
 - Engineering fluid dynamics, microfluidics, bio-fluids
 - Environmental sciences mineral structure, materials damage, coastal modeling
 - Numerical analysis, software engineering and applied e-science
 - Major codes produced in all areas



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 GAMESS-UK: ab initio molecular electronic structure program for performing SCF-, MCSCF- and DFT-gradient calculations, together with a variety of post Hartree Fock techniques. Integrated QM/MM modelling. (261 [31] users) CCP1 (CCP3)
 DL POLY: general purpose molecular dynamics code, replicated/ distributed data

- DL_POLY: general purpose molecular dynamics code, replicated/ distributed data, NVT, NPT, NST, NVE thermodynamic ensembles, MTS and RESPA algorithms, Ewald summation for electro-statics. (540 [162] users) CCP5
- DL_MESO: general purpose Lattice Boltzmann, Dissipative Particle Dynamics and Smooth Particle Hydrodynamics code. (73 [61] users) CCP5 (CCP12)
- CRYSTAL: 1D, 2D, 3D periodic Gaussian, Hartree-Fock, total energy, forces. Under continuous development by the CMS group at DL and the University of Turin since 1974 (CRYSTAL 2003 - 243 [63] users) CCP3 (CCP1)
- CASTEP: The Cambridge Serial Total Energy Package plane wave DFT calculation of the total energy, forces and stresses in a 3D-periodic system. (150 users) UKCP, CCP3, CCP9
- DL_EXCURV: Analysis of exafs data from synchrotron radiation sources (540 users) CCP3, LighTneT
- Plus many others e.g., POLCOMS, FLITE3D, PCHAN, SIC-LMTO, THOR,

[] Licences Issued in 2005









Science and Innovation in the Campus Model

- In the "Next Steps" document published in March 2004, the UK Government called into existence two new Science and Innovation Campuses at Daresbury and Harwell
- DSIC and HSIC will be the focus of the government's investment in large scale scientific infrastructure
- They will be the key vehicle supporting the Government's Knowledge Transfer agenda

• The Campus model brings together a National Laboratory with the best universities and high-tech industry.

• For the computational sciences, this is a unique environment in which to take the field to a much higher level in the UK.

	ce and innovation nework 2004-2014:
ivestment iran	next steps
	March 2006

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The International Review of UK Research using HPC, 2005

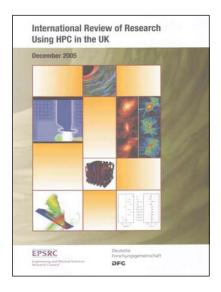
In 2005 EPSRC commissioned an International Review of Research Using HPC in the UK, conducted by the German Research Council DFG.

The Review Panel was chaired by Horst Simon (Director of NERSC at Berkeley, USA) and involved a distinguished group of world experts.

The Panel wrote "[UK research] in many areas is of the highest standing and competitive at the international level."

But they made a number of recommendations to enable the UK "to maintain its position at the forefront of research using HPC."

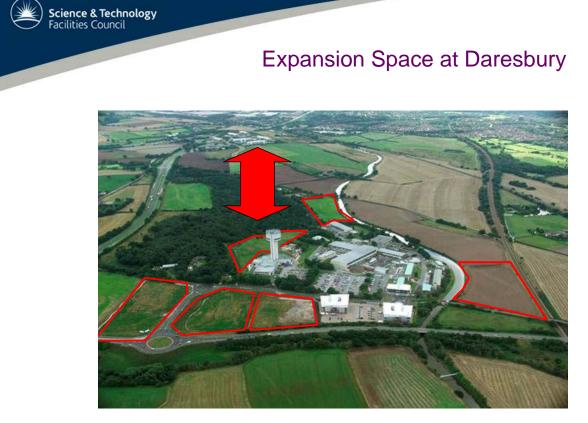
In particular, they noted the lack of a focused national "all-embracing computational science community", despite much excellent collaboration within specific sub-fields of the discipline.





The Research Centre Model

- Following the model of the very successful Cockcroft Institute for accelerator science, can future scientific activities at DSIC be structured around a set of world class Research Centres?
- These Centres should:
 - Build on established world-class capabilities in STFC to achieve critical mass
 - Align with and support STFC's scientific strategic objectives
 - Implement the "dipole" Science and Innovation Campus model, linking DSIC and HSIC in a direct way
 - Involve the right world-class partners from (local) academia and play a key role in implementing the strategies of partner organisations
 - Have a clear international status and conduct international programmes
 - Play a strong role in training young scientists and engineers in scarce skills
 - Contain specific knowledge transfer activities that connect clearly with DSIC Innovation Centres
- We are developing plans for the Hartree Centre a home for CSE and HPC in the UK and a platform for an internationally leading activity



NWDA "Key NW Strategic Site"



The Role of the Hartree Centre

- The UK has lots of very good computational research but it is fragmented and its impact is diluted.
- The UK computational sciences community needs a focal point if it is to be fully recognised as a world leader the Hartree Centre will be this focus.
- It will enable the UK to lead in European opportunities and to be a full partner in many US initiatives. (Japanese initiatives?)
- The Centre will act as forum within which the scientists themselves can discuss, develop and articulate policy for computational research independently from the funding agencies – cf the Report of the 2005 International Review.
- The Centre will form alliances with h/w and s/w industry to enable UK researchers to access novel technology early and with the minimum of pain.
- It will provide software engineering support for its partners



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The Vision

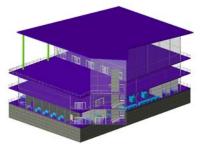
The Hartree Centre will be a new kind of Computational Sciences institute for the UK that will:

- stimulate a step change in modeling capabilities for strategic science themes;
- multi-disciplinary, multi-scale, effective and efficient simulation;
- be amongst the best in the world -ORNL, NCSA, SDSC,.. in scale and quality;
- partner with the best academic, government agency and industrial groups both national and international;
- couple computational science and HPC facilities strongly to large experimental facilities;
- build capacity with a much expanded training programme;
- seek to host European Computational Science and Engineering research organisations – eg CECAM, psi-K, ..
- act as a focus for the UK community and enable it to take an international lead in the field;
- have at its heart the collaborative development, support and exploitation of scientific applications software – this is the key to real scientific and economic impact and will be Hartree's essential driver.



The Hartree Centre – will contain

- Facility
 - 10,000 square feet machine room
 - 10 MW power
 - £10M systems / two year cycle
 - Other commodity and capability academic and commercial facilities
 - Training facilities, visualisation, access grid,
 - Host for psi-K and emerging European cyberinfrastructure
 - £45M of capital and £1M running costs for 5 years
- Partners
 - CSED and e-science @ STFC
 - UK academic partners colocate tenured staff, PDRAs, research students
 - Other Public Sector Research Establishments
 - International Partners: NCSA, ORNL, PNNL, NIH, ...
 - Hardware/ system technology providers DSIC
 - Commercial software vendors DSIC
 - Industrial end users involved in R&D portfolio
 - £50M portfolio of R&D and technical projects







The Hartree Centre is a REAL Institute, not a Virtual One!

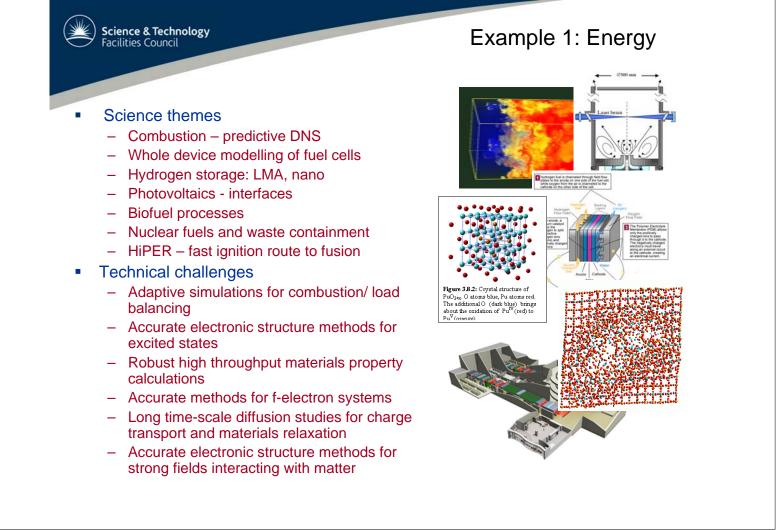
The current plan involves a large 3 – 4 story building. The basement level will be a purpose-designed modern machine room with ample floor space, power supplies and cooling.

> Staff from partner organisations will be physically co-located in the Centre, so that critical mass will be actually, not virtually, achieved.



STFC's Strategic Science Themes

- Energy e.g. simulation & modelling of combustion, nuclear fuel stocks, containment, fuel cells,
- Biomedical science e.g. predicitive models of the cell, organs, systems, organisms
- Environment e.g. coupled models providing insight into extreme events and uncertainty
- Functional materials e.g. computational nanoscience, device simulation etc
- Modelling facilities accelerators, lasers, neutron sources, fusion and theory of their experiments
- Particle Physics e.g. computational approaches to field theory in particle physics (QCD etc)
- Laboratory astrophysics e.g. simulation of galaxy formation





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Science themes

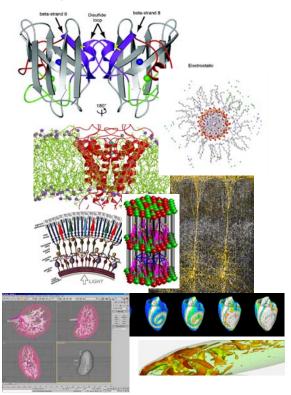
SimCell -

- computational enzymology, protein structure, dynamics and function, membrane transport
- Three dimensional spatial/ temporal models of cells for reaction/ diffusion intercelluar interactions
- Development of 'continuum' cell models for use in SimOrg

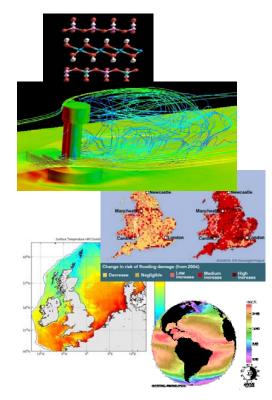
SimOrg -

- development of continuum and point based descriptions of tissues, organs, systems and organsisms: eye, microcortex, kidney, heart, circulation, ..
- Technical challenges
 - Scalability as many time steps/second
 - Coarse graining to get beyond microsecond timescales
 - Model characterisation structure and properties of many different cell types
 - Multidisciplinary simulations fluid/ solid, adaptive physics and chemistry
 - Connectivity of cells especially in cognitive/ nervous system

Example 2: Lifesciences



Example 3: Environment



Science themes

Facilities Council

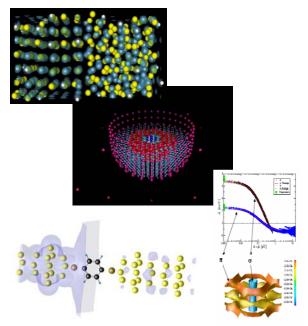
Science & Technology

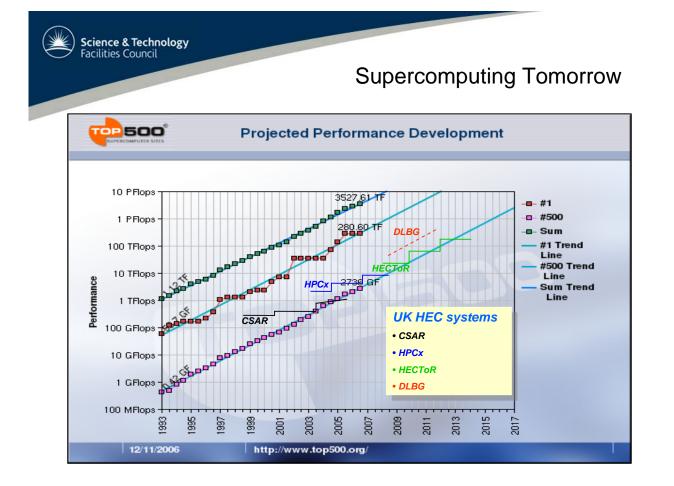
- Understanding the phase diagram and properties of water containing and carbon sequestration minerals
- to enable higher resolution (accuracy and regional detail and more accurate simulations (heatwaves, storms, flooding)
- More physics and chemistry
- Quantifying climate variability and uncertainty
- Global shelf edge modelling and its effect on global climate change
- Technical Challenges
 - address scalability issues in Met Office Unified Model code in research project involving University Manchester, STFC and IBM
 - Load balance multiphysics and adaptive physics/ chemistry
 - POLCOMS



Example 4: Functional Materials

- Science themes
 - Predictive capability for the phase diagram of complex materials
 - catalysts
 - characterisation of nanostructures
 - using spin to provide a new generation of functional devices
 - molecular electronics materials
 - superconducting materials
- Technical challenges
 - new O(N) methods
 - Robust high-throughput methods
 - Treatment of correlation: TD-DFT, MBPT-GW, Quantum Monte Carlo, Self-interaction correction, dynamic correlations







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Technology

- General purpose architectures performance/ power/ affordability
- Architectures are now more diverse; no single architecture fits all problems; one size does not fit all!
- Computing technology must be coupled to mission achieving real scientific impact from HPC
- Partnership with Technology Provider to position UK at the leading edge of massively parallel supercomputing:
 - Architectures that can scale cost-effectively (including footprint and running costs) to hundreds of thousands of processors - exascale challenge
- Develop a distinctive STFC approach to computational research, complementary to EPSRC's:
 - not a general purpose facility; deployed on selected high impact projects especially energy, bioscience, materials and environment
 - closely coupled to international portfolio of experimental facilities
 - new generation of simulation codes that scale to very large numbers of processors
 - Run as beamlines 2 months dedicated 10²¹ flop simulations
- Scale of system:
 - Iniital system: 100-200 Tflops, Second system:1-2 Pflops
 - For selected problems this needs to represent a step change in cost-effectiveness over commodity and general purpose systems

- Science & Technology Facilities Council Technology Themes – Realising the Potential Scalable Algorithms (SA) load balance on up to 10⁶ cores adaptive resolution and adaptive physics/ chemistry O(N) algorithms Scale with number of variables – low prefactor Management of Memory Hierarchy (MH) Numerically intensive algorithms, optimise memory access for comms buffers or memory bandwidth Fault Tolerant Computing (FT) - FT-MPI, applications level Data Management and Visualization (DM) - Parallel I/O, database queries, on the fly visualisation Performance Analysis (PA)
 - Develop strategic relationship with developers debuggers/ optimisers/ languages/ ..
 - Software Engineering (SE) Assist developers in adopting modern tools and best practices



Centre for Earth Systems Intelligence (CESI) A new centre for environmental modelling to be based at DSIC

Proposed Offerings

- On demand service for weather models, water management
- Optimization of thermal efficiency in data centers
- Services offerings such as materials characterization
- Services offerings such as molecular design for nano-filtration, biofuels

Additional applications/offerings

- Energy grid optimization
- Nuclear reactor/fuel modeling
- Water network optimization
- Carbon footprint optimization
- Material science (for example creating new PV materials or filtration and battery membranes)

Computational Modeling to support

- Big Green Innovations portfolio
- Energy & Utilities nuclear modeling and grid modeling
- Green Data Centers thermal modeling and optimization

STFC - Daresbury Laboratory, Hadley Centre for Climate Prediction & Research, Lloyds Insurance, Walker Institute for Climate Research, Proudman Oceanographic Laboratory, North West Development Agency, IBM **Research & IBM Global Business** Services, DEFRA, ..

£1M pa turnover -





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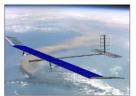
Integrate high fidelity simulation into the supply chain and lifecycle analysis

- Conception
- Requirements capture
- Design performance/ optimisation
- Acceptance
- Production
- Maintenance Through-life support
- Upgrade
- Obsolescence
- Disposal

Virtual Engineering Centre

North West Aerospace Alliance, BAE Systems, Rolls Royce, Airbus, Universities of Manchester, Lancaster and Liverpool, STFC Daresbury Laboratory and NW-GRID

£1M pa turnover









Knowledge Centre for Materials Chemistry

- Energy and Sustainability hydrogen economy, biofuels, photovoltaics, process route selection, design methodology
- Electronics and Photonics organic and inorganic semiconductors, dielectrics and metals, devices, sensors, spintronics
- Complex Materials membranes, catalysis, gas storage, smart packages, nanoparticles, biomaterials
- Biologically Relevant Materials regenerative medicine, peptides, drug delivery
- Formulated Products multicomponent products, direct write, soft solids, discovering new solid forms, fire retardant

World class capabilities in the universities of Bolton, Liverpool and Manchester, and CSE at Daresbury Laboratory.

The Centre will be managed by an independent Knowledge Transfer Team whose role will be to foster and grow industrial collaborations in the NW and beyond.

£5M pa turnover

The NW will remain competitive and attractive in the area despite a strong challenge from the Far East. We estimate the creation of over 300 new jobs: 28 in the Centre; 50 in 10 new spin-out companies; 250 in the region's chemistry using industries.



- access to STFC technology e.g. Blue Gene, technology
- 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
- joint supervisors, as teachers, examiners ...
- development of computational science courses
- training programmes
- CSE/ HPC marketing activities facilities, codes and solutions
- environment for HPC/ CSE spin-out activities
- development of new industrial Consortia



Current Status

Bid into CSR 2007 as part of Campus Project £30M building plus two £10M 'experimental' systems - £50M capital

Bid for £2M pa STFC Core Funding for:

- code development grants line
- support for facilities
- computing infrastructure

Complemented by bids for specific projects:

7 workshops covering key science themes focussing on petascale and exa-scale applications

KE activities:

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- Virtual Research in Engineering Centre
- Centre for Earth Systems Intelligence
- Knowledge Centre for Materials Chemistry
- Vendor discussions

Build Hartree Centre - 2 years from approval - April 2010 at earliest

Phase 1 system install (200-400TF) – April 2010 Phase 2 system install (1-2 PF) – April 2012



Conclusions

- The CCP's provide a vibrant long term home for the development of CSE applications codes
- Staff support from CSED@STFC has been critical to this vision
- CSE is a growing activity within STFC
- The Hartree Centre will provide a home for the UK computational effort



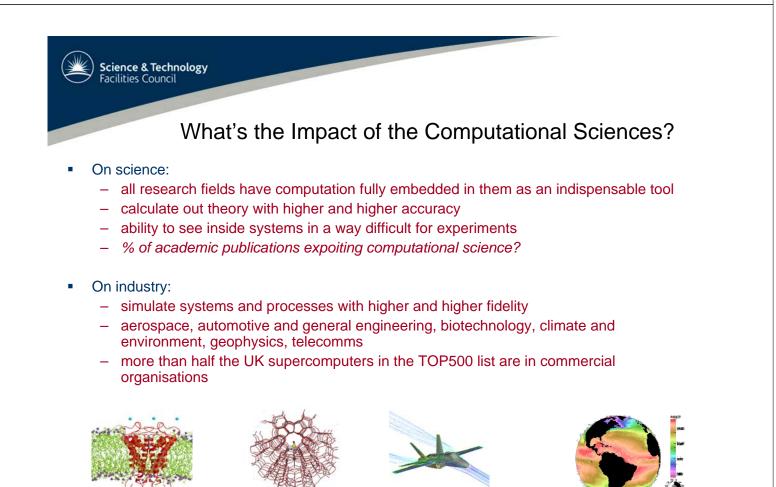
What is Computational Science?

- Do theory, make mathematical models
- Write programs
- Use programs to do science
- Make programs available to university colleagues and support them
- Make programs run quickly on the fastest machines around

Solving the Schrodinger equation, Newton's equations, Navier-Stokes equations, etc for ever more complicated and realistic models.



Figure 1. The spectrum of computing resources.





"Computational science is now indispensable to the solution of complex problems in every sector, from traditional science and engineering domains to such key areas as national security, public health and economic innovation"

President's Information Technology Advisory Committee (2005)

"[The computational sciences] today serve to advance all of science and engineering, and many areas of research in the future will only be accessible to those with access to advanced computational technology"

International Review of Research Using HPC in the UK (2005)

So the UK cannot afford not to have a world-leading computational sciences activity and community.

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Computational Research is a Big Business

	Project Cost (M£)	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012
CSAR	25	4.2	4.2	4.2	4.2	2.1						
HPCx	54		9.0	9.0	9.0	9.0	9.0	9.0				
HECToR	110						9.2	18.3	18.3	18.3	18.3	18.3
CoH	100									16.7	16.7	16.7
Annual Spend	(M£)	4.2	13.2	13.2	13.2	11.1	18.2	27.3	18.3	35.0	35.0	35.0

	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012
SRIF 1	17.5	17.5									
SRIF 2			22.5	22.5							
SRIF 3					19.0	19.0					
SRIF 4??							??	??	??	??	??
Annual Spend	(M£) 17.5	17.5	22.5	22.5	19.0	19.0	??	??	??	??	??

ESFRI Roadmap

	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012
High-End Infrastructure							66.7	66.7	66.7	66.7	66.7
Medium Level Infrastructure						50.0	50.0	50.0	50.0	50.0	50.0
Maintenance & Upgrades						50.0	100.0	100.0	100.0	100.0	100.0
Software Development						50.0	50.0	50.0	50.0	50.0	50.0
Annual Spend (M€)	0.0	0.0	0.0	0.0	0.0	150.0	266.7	266.7	266.7	266.7	266.7

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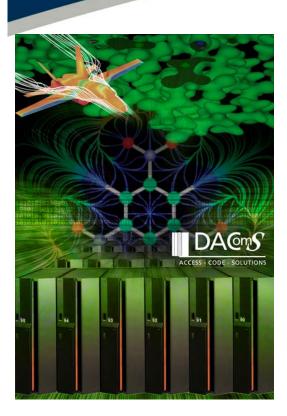
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- The Aeronautical Journal, Volume 111, Number 1117 (March 2007), UK Applied Aerodynamics Consortium, Special Edition.
- Last 5 years metrics:
 - 67 grants of order £13M
 - 422 refereed papers and 275 presentations
 - Three senior staff have joint appointments with Universities
 - Seven staff have visiting professorships
 - Six members of staff awarded Senior Fellowships or Fellowships by Research Councils' individual merit scheme
 - Five staff are Fellows of senior learned societies





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Working with Industry



CSE Department has established DAComS as its knowledge transfer brand – with a presence in the Daresbury Innovation Centre



ACCESS

HPCx NWGRID

Commodity Technology

CODE

Bespoke STFC

FFC Commercial

SOLUTIONS

CSE knowledge, skills and expertise applying above to solve problem

PRODUCT

Access + Code + CSE delivering the solutions