The Collaborative Computational Projects (CCPs)

Dr Adrian Wander
Computational Science and Engineering
Department
STFC Daresbury Laboratory
Daresbury, Warrington, WA4 4AD
UK

a.wander@dl.ac.uk  http://www.cse.scitech.ac.uk

Overview

- 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

- scale of code development
- scientific software is a generic tool
- ensuring longevity and exploitation

The CCP model
HEC consortia

CCP1: Electronic Structure of Molecules (P Knowles)
CCP2: Continuum States of Atoms and Molecules (E Armour)
CCP3: Computational Studies of Surfaces (S Crampin)
CCP4: Protein Crystallography (J Naismith)
CCP5: Computer Simulation of Condensed Phases (M Rodger)
CCP6: Molecular Quantum Dynamics (S Althorpe)
[CCP7: Astronomical Spectra (Prof D Flower)]
CCP9: Electronic Structure of Solids (J Annett)
CCP11: Biosequences and Function (D Gilbert)
CCP12: High Performance Computing in Engineering (S Cant)
CCP14: Powder Diffraction (J Cockcroft)
CCPN: NMR in structural biology (E Laue)
CCPB: Bio-molecular Simulation (C Laughton)
CCPP: Plasma Physics CCP (tba)

13 CCPs ~ 370 groups
53 HPC Consortia ~ 150 groups in UK
EU networks ~ 50 groups in EU
HPCx ~ 900 users
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

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?
Scientific Highlights …

- **Journal of Materials Chemistry** 16 no. 20 (May 2006) - issue devoted to HPC in materials chemistry (esp. use of HPCx); CCP1, CCP3, Mat Sci Consortium

- **Phys. Stat. Sol.(b)** 243 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** 32 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** 63 part 1 (Jan 2007) - proceedings of the CCP4 Study Weekend on protein crystallography. CCP4


---

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)
Science and Technology Facilities Council (STFC)

- Supports large scale experimental facilities and centres of technical excellence for the UK Research Community
  - Neutron sources
  - Lasers/ light source science
  - HPC, CSE and e-science
  - Engineering, instrumentation, accelerators
  - Funds particle physics and astronomy research

- Formed from the merger of CCLRC and PPARC in 2007
- Operates out of Swindon (Head Office), Rutherford, Daresbury, Edinburgh, Chilboton and Selby
- Budget of order £735M pa – a big organisation
- A young organisation reviewing what is strategically important and what it is good at

  World class activities in high-performance computing and computational science and engineering

Research Councils

- UK Government
  - DIUS
  - Office of Science & Innovation

- ESRC
- AHRC
- EPSRC
- STFC
- NERC
- BBSRC
- MRC

- Daresbury Laboratory
- Computational Science & Engineering Department
- Rutherford Appleton Laboratory
How Important is the Computational Science Community to STFC?

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

**STFC User Trends**

- CLF
- Engineering
- SSTD
- PP
- ISIS
- SRS
- Computing

Major funded activities:
- Research,
- Applications development and support – CCPs and HEC Consortia
- Compute and data facilities and services – HPCx
- 80 staff - £7M pa turnover
- International collaborations

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

**Mission:** “Ensuring that UK researchers benefit from the best computational methods and techniques”

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

All underpinned by an R&D and support programme in technical computing
Growth of the CSED

We're heading for ~100 staff split 70:30 between Daresbury and RAL

Trends in Staff Numbers

<table>
<thead>
<tr>
<th>Year</th>
<th>Planned SY</th>
<th>Headcount</th>
</tr>
</thead>
<tbody>
<tr>
<td>1990/91</td>
<td>30</td>
<td>30</td>
</tr>
<tr>
<td>1992/93</td>
<td>35</td>
<td>35</td>
</tr>
<tr>
<td>1994/95</td>
<td>40</td>
<td>40</td>
</tr>
<tr>
<td>1996/97</td>
<td>45</td>
<td>45</td>
</tr>
<tr>
<td>1998/99</td>
<td>50</td>
<td>50</td>
</tr>
<tr>
<td>2000/01</td>
<td>55</td>
<td>55</td>
</tr>
<tr>
<td>2002/03</td>
<td>60</td>
<td>60</td>
</tr>
<tr>
<td>2004/05</td>
<td>65</td>
<td>65</td>
</tr>
<tr>
<td>2006/07</td>
<td>70</td>
<td>70</td>
</tr>
</tbody>
</table>

Application Codes

- 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, 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, LightTneT
- Plus many others e.g., POLCOMS, FLITE3D, PCHAN, SIC-LMTO, THOR,

Licences Issued in 2005
Facilities

The Hartree Centre A New CS&E Institute on the Daresbury Science and Innovation Campus
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.**

---

**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

Expansion Space at Daresbury

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

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 cyber-infrastructure
  - £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. predictive 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

Example 1: Energy

- Science themes
  - Combustion – predictive DNS
  - Whole device modelling of fuel cells
  - Hydrogen storage: LMA, nano
  - Photovoltaics - interfaces
  - Biofuel processes
  - Nuclear fuels and waste containment
  - HiPER – fast ignition route to fusion
- Technical challenges
  - Adaptive simulations for combustion/ load balancing
  - Accurate electronic structure methods for excited states
  - Robust high throughput materials property calculations
  - Accurate methods for f-electron systems
  - Long time-scale diffusion studies for charge transport and materials relaxation
  - Accurate electronic structure methods for strong fields interacting with matter
Example 2: Lifesciences

- **Science themes**
  - SimCell –
    - computational enzymology, protein structure, dynamics and function, membrane transport
    - Three dimensional spatial/temporal models of cells for reaction/diffusion intercellular interactions
    - Development of ‘continuum’ cell models for use in SimOrg
  - SimOrg –
    - development of continuum and point based descriptions of tissues, organs, systems and organisms: 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 3: Environment

- **Science themes**
  - 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

Supercomputing Tomorrow

**Projected Performance Development**

- CSAR
- HPCx
- HECToR
- DLBG

**UK HEC systems**

- CSAR
- HPCx
- HECToR
- DLBG
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 – $10^{21}$ flop simulations
- Scale of system:
  - Initial 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

Technology Themes – Realising the Potential

- Scalable Algorithms (SA)
  - load balance on up to $10^6$ 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 comm 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
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

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

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 -

Virtual Engineering Centre

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

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.

The University Partnerships

What could universities get from Hartree Centre:

- 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 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:
- 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 Schrödinger equation, Newton's equations, Navier-Stokes equations, etc for ever more complicated and realistic models.

What’s the Impact of the Computational Sciences?

- On science:
  - all research fields have computation fully embedded in them as an indispensable tool
  - calculate out theory with higher and higher accuracy
  - ability to see inside systems in a way difficult for experiments
  - % of academic publications exploiting computational science?

- On industry:
  - simulate systems and processes with higher and higher fidelity
  - aerospace, automotive and general engineering, biotechnology, climate and environment, geophysics, telecomms
  - more than half the UK supercomputers in the TOP500 list are in commercial organisations
“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.

Computational Research is a Big Business

### UK Supercomputing

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>CSAR</td>
<td>25</td>
<td>4.2</td>
<td>4.2</td>
<td>4.2</td>
<td>4.2</td>
<td>2.1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HPCx</td>
<td>54</td>
<td>9.0</td>
<td>9.0</td>
<td>9.0</td>
<td>9.0</td>
<td>9.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HECToR</td>
<td>110</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>9.2</td>
<td>18.3</td>
<td>18.3</td>
<td>18.3</td>
<td>18.3</td>
</tr>
<tr>
<td>CoH</td>
<td>100</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Annual Spend (M£)</strong></td>
<td>4.2</td>
<td>13.2</td>
<td>13.2</td>
<td>11.1</td>
<td>18.2</td>
<td>27.3</td>
<td>18.3</td>
<td>35.0</td>
<td>35.0</td>
<td>35.0</td>
<td>35.0</td>
</tr>
</tbody>
</table>

### UK Mid-range infrastructure

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>SIRF 1</td>
<td>17.5</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SIRF 2</td>
<td></td>
<td>22.5</td>
<td>22.5</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SIRF 3</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>19.0</td>
<td>19.0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SIRF 4??</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Annual Spend (M£)</strong></td>
<td>17.5</td>
<td>17.5</td>
<td>22.5</td>
<td>22.5</td>
<td>19.0</td>
<td>19.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### ESFRI Roadmap

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>High-End Infrastructure</td>
<td>66.7</td>
<td>66.7</td>
<td>66.7</td>
<td>66.7</td>
<td>66.7</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Medium Level Infrastructure</td>
<td>50.0</td>
<td>50.0</td>
<td>50.0</td>
<td>50.0</td>
<td>50.0</td>
<td>50.0</td>
<td>50.0</td>
<td>50.0</td>
<td>50.0</td>
<td>50.0</td>
<td>50.0</td>
</tr>
<tr>
<td>Maintenance &amp; Upgrades</td>
<td>50.0</td>
<td>100.0</td>
<td>100.0</td>
<td>100.0</td>
<td>100.0</td>
<td>100.0</td>
<td>100.0</td>
<td>100.0</td>
<td>100.0</td>
<td>100.0</td>
<td>100.0</td>
</tr>
<tr>
<td>Software Development</td>
<td>50.0</td>
<td>50.0</td>
<td>50.0</td>
<td>50.0</td>
<td>50.0</td>
<td>50.0</td>
<td>50.0</td>
<td>50.0</td>
<td>50.0</td>
<td>50.0</td>
<td>50.0</td>
</tr>
<tr>
<td><strong>Annual Spend (M£)</strong></td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>150.0</td>
<td>266.7</td>
<td>266.7</td>
<td>266.7</td>
<td>266.7</td>
<td>266.7</td>
<td>266.7</td>
</tr>
</tbody>
</table>
Scientific Highlights …

- *Journal of Materials Chemistry* 16 no. 20 (May 2006) - issue devoted to HPC in materials chemistry (esp. use of HPCx);
- *Phys. Stat. Sol.(b)* 243 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);
- *Molecular Simulation* 32 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);
- *Acta Crystallographica Section D* 63 part 1 (Jan 2007) - proceedings of the CCP4 Study Weekend on protein crystallography.

**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 Fellowship or Fellowships by Research Councils’ individual merit scheme
- Five staff are Fellows of senior learned societies

**International Scene**

**Collaborations with the USA**

**CCP Participation in the UK**

**CCP Collaborations in Europe**

**TeraGrid collaboration**
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
- Commercial

**SOLUTIONS**
- CSE knowledge, skills and expertise applying above to solve problem

**PRODUCT**
- Access + Code + CSE delivering the solutions