

Software for the Future – 31st May 2012

Introduction

EPSRC have supported software activities for a number of years and through a variety of [mechanisms](#). In January 2012, we published our [Software as an Infrastructure strategy](#) which followed on from these activities, their outputs and a workshop held in October 2011.

Background

The workshop had two aims: one was to map the current UK activities in software and the other was to determine the needs for support for software in the future. Given this dual aim, the workshop was run in two parts.

The morning session was dedicated to discussion of the activities that are currently taking place in software and attempting to work out how they linked with each other. Attendees at the morning session were invited because they had current funding from EPSRC or were involved in activities supported by other funders.

The afternoon session was attended by those from the morning and a selection of people based on applications submitted to a [call for participants](#). Those chosen for the afternoon aimed to be representative of the broad community in terms of expertise, applications and techniques.

Activities and outputs on the day

The task of the morning attendees was to create a map of the software activities that are currently taking place in the UK (or that the UK links into internationally). This activity led to the composition that is shown at the top of [Annex 1](#). Most of the activities on the map have been listed, along with an accompanying description. The map that was created at the workshop has also been redrawn graphically. The map represents activities with a fair amount of critical mass so some of the smaller, more discreet activities that were originally listed or funders themselves are not represented in the activities map. There are links throughout the map and the list of activities in order to lead the reader through everything.

Once the map had been created, the morning attendees used it to identify gaps in the type of software provision. This led to the development of eight areas that warranted further discussion in the afternoon.

- 1: Career Development
- 2: Co-ordination of Activities
- 3: Engagement and coordination with other funders (incl. TSB)
- 4: Training
- 5: Putting the middle into the pyramid
- 6: Widening Participation
- 7: Preparing software for the next generation of computer systems
- 8: International Engagement

Afternoon attendees were able to choose which session they attended. The International engagement session did not attract interest and as session 7 was oversubscribed this was split in to two. Each session was led by someone who had attended the morning part of the workshop and the groups were tasked with filling out a pre-designed form with the aim of capturing where investment was needed in the future. These forms are presented, as they were handed in following the workshop, in [Annex 2](#).

A list of all attendees to the workshop is in [Annex 3](#).

Post-workshop work

Following the workshop, EPSRC assimilated the outputs and has used this information to inform future activities. There is EPSRC commentary that has been added alongside each of the inputs to the forms in Annex 2. The information that was gathered about training needs has been fed into the team managing the CDTs. There has also been discussion with the Technology Strategy Board about working with them on their [Energy Efficient Computing Emerging Technology Theme](#). EPSRC is using the outputs of the workshop to help inform a large call that will be focussed around developing software for future applications. This is due to be released in August 2012.

Next steps

EPSRC will continue to develop its strategy in line with the Software as an Infrastructure strategy. Other funders such as other Research Councils, JISC, the Technology Strategy Board and overseas organisations are important in growing and implementing this strategy and will be engaged with appropriately. Community engagement is integral to moving the strategy forward and EPSRC will continue to cultivate the links already in place and grow new relationships.

Annex 1: Activities

Map of activities



Photo courtesy of Nick Higham, University of Manchester

List of activities

CCPP
Links to industry and Technology Strategy Board , SESP
The study of plasma physics covers a huge range of scales and applications. It is core to the development of laboratory experiments such as fusion power, new light sources and the next generation of particle accelerators. On the largest scales it is fundamental to our understanding of astrophysics. CCPP was established in 2007 with the aim of pooling the collective expertise across these disparate subjects and developing core plasma physics simulation codes, and training packages, for UK science.
Jikes RVM
Jikes RVM (Research Virtual Machine) provides a flexible open testbed to prototype virtual machine technologies and experiment with a large variety of design alternatives. Jikes RVM runs on many platforms and advances the state-of-the-art of virtual machine technologies for dynamic compilation, adaptive optimization, garbage collection, thread scheduling, and synchronization. A distinguishing characteristic of Jikes RVM is that it is implemented in the Java™ programming language and is self-hosted i.e., its Java code runs on itself without requiring a second virtual machine. Most other virtual machines for the Java platform are written in native code (typically, C or C++). A Java implementation provides ease of portability, and a seamless integration of virtual machine and application resources such as objects, threads, and operating-system interfaces.
NeuroHub (JISC)
Links to e-Research South
This project will develop a set of sustainable tools and framework that will allow neuroscientists to efficiently and effectively use existing e-Infrastructure and by doing so will enable a more productive research cycle, streamlining the laboratory experience from conception of experiment to publication of the research results. The framework and tools will be the product of in depth user requirements analysis, adaptation of existing software, development of key missing components and a tight collaboration between neuroscientists, technologists and resource providers at three HEIs. The collaboration leverages the e-Research South consortium and builds on both a strategic regional activity and University strategy

that will provide sustainability beyond the lifetime of the project. The research outputs will include open source software as well as best practice guides and training material.

New techniques for greater scalability

Links to [NAIS](#), [ASEArch](#), [NA network](#)

Activities working towards making hardware more asynchronous for codes such as LINPAC and Monte Carlo

[NSCCS – National service for computational chemistry software](#)

Links to [Diamond](#)

The EPSRC UK National Service for Computational Chemistry Software (NSCCS) at Imperial College London provides access to software, specialist consultation, computing resources and software training to support UK academics working across all fields of chemistry.

[Research tools \(JISC\)](#)

Links to [SSI](#)

The strand builds on work undertaken by the [Virtual research environment](#) (VRE) and [Research infrastructures programmes](#). The VRE programme funded work to help researchers from all disciplines to work collaboratively by managing the increasingly complex range of tasks involved in carrying out research on both small and large scales. VREs take a coherent approach to joining up tools to serve particular or generic aspects of the research lifecycle.

The Research infrastructure programme supported development and embedding of the underlying infrastructure that enables the use of research tools. A particular focus was grid and cloud computing and the Research tools strand will continue some of these activities.

[Materials Chemistry HECToR Consortium \(MCC\)](#)

Links to [UKCP](#), [non equilibrium flow programme grant](#)

The HPC Materials Chemistry Consortium exploits the latest developments in HPC technologies, in a wide ranging programme of development, optimisation and applications studies aimed at modelling and predicting the structures, properties and reactivities of functional materials, including catalysts, ceramics, minerals and molecular materials. The programme embraces both large scale simulations based on forcefields and electronic structure techniques employing both Density Functional Theory, Hartree Fock and hybrid techniques. Strong emphasis is placed on code development and optimisation for MPP platforms while several applications highlight systems of industrial importance. There is strong symbiosis between the modelling studies of the consortium and experimental programmes.

[Diamond \(Dawn/GDA\)](#)

Links to [e-Research South](#), [NSCCS](#), [SKA](#)

Diamond Light Source is the UK's national synchrotron science facility and uses DAWN and GDA as software tools.

DAWN is a high quality generic tool for scientific data analysis. It is developed by and for the synchrotron community foremost but has strong overlap with other communities like neutron scattering, photon science and any scientific communities with similar needs.

The mission of GDA is to create, as a community, a customisable Java software framework to operate experiments on synchrotron facilities. It will contain: hardware control (directly or via any control system); data acquisition logic; a graphical user interface; scripting tools; and data visualization and analysis tools.

Tier 2 centres

Links to [e-Research South](#), [Diamond](#), [DiRAC](#)

EPSRC has funded hardware at a number of regional sites across the UK. There are:

- [e-Infrastructure South \(a consortium of the Universities of Oxford, Bristol, Southampton and UCL\)](#)
- [A Midlands Centre of Excellence for High Performance Computing \(Universities of Loughborough and Leicester\)](#)
- [West of Scotland Supercomputing Centre of Academia and Industry \(Universities of Strathclyde, Glasgow, Glasgow Caledonian, West of Scotland and Stirling\)](#)
- [E-Infrastructure Interconnectivity \(Universities of Manchester, Durham, Lancaster, Leeds, Liverpool, Newcastle, Sheffield and York\)](#)
- [MidPlus: A Centre of Excellence for Computational Science, Engineering and Mathematics \(Universities of Warwick, Birmingham and Nottingham\)](#)

e-Research South

Links to [JISC research tools](#), [Diamond](#), [tier 2](#), [DiRAC](#), [Neuro Hub](#)

The e-Infrastructure South consortium is formed through a partnership of the Universities of Bristol, Oxford, Southampton and UCL. Formed in 2011, the consortium has the express aim of exploring and exploiting opportunities for the co-development and sharing of e-infrastructure capabilities (hardware, applications software, user support services and people and skills) across the founding institutions and through linkages with other academic and industrial partners across the South of England.

UK Car Parrinello (UKCP) HECToR consortium

Links to [non equilibrium flow programme grant](#), [CCP Forge](#), [CCP9](#), [CCP NC](#), [MCC](#)

The UK Car-Parrinello Consortium is an association of research groups collaborating on the first-principles computer simulation of condensed matter. The aim is to use the creativity and strength of collaboration and shared expertise to produce outstanding science and simulation software.

UK Turbulence consortium HECToR consortium (UKTC)

Links to [ASEArch](#), [CCP12](#), [HECToR CSE](#), [non equilibrium flow programme grant](#)

The UK turbulence consortium is a group of academics and researchers from across eight universities, committed to undertaking high quality, world leading turbulence simulation and scientific research. They use high performance computing systems, such as HECToR, to investigate fundamental aspects of turbulence problems using numerical simulations. Cases include transitional and fully developed turbulent flows in canonical and complex geometries, with relevance to a wide range of engineering, environmental/geophysical and biological applications.

Non-Equilibrium Fluid Dynamics for Micro/Nano Engineering Systems Programme Grant

Links to [UKCP](#), [CCP12](#), [MCC](#), [UKTC](#), [CCPQ](#)

This research is about simulating and designing the engineering flow systems that will form a major part of the responses to health, transportation, energy and climate challenges that the world faces over the next 40 years. This cross-disciplinary research programme targets the unconventional fluid dynamics that is key to innovating in these visionary applications and aims to deliver a comprehensive new technique for simulating mixed equilibrium/non-equilibrium fluid dynamics at the nano and micro scale.

CCPQ: Quantum phenomena

Links to [ASEArch](#), [emerging software technology](#), [non equilibrium flow programme grant](#), [SLA](#)

CCPQ is a collaborative computational project with the original objectives (as CCP2) of developing theoretical techniques and computer programs to describe collisions between projectiles such as electrons, positrons or photons and atomic or molecular targets. Over the years these objectives have

expanded to include atoms and molecules in strong (long-pulse and attosecond) laser fields, low-energy interactions of antihydrogen with small atoms and molecules, cold atoms, Bose-Einstein condensates and optical lattices. The project involves research scientists from UK universities and government laboratories as well as scientists from Germany, Italy, Japan and US. In late 2011, CCP2 was 'reborn' as CCPQ, taking in network activities, code curation and related molecular research such as molecular wavepacket dynamics, ultracold molecule formation and cold chemistry, from CCP6.

[CCPi: Tomographic imaging and visualisation](#)

Links to [ASEArch](#), [CCP Forge](#), [SLA](#)

Computed Tomography (CT) is a powerful non-destructive evaluation (NDE) technique for producing 2-D cross-sections and 3-D images of an object from a series of 2D projections (shadowgraphs). Critical to the process is the computer algorithms that are able to reconstruct the 3D images from many (often over a thousand) shadowgraphs. There are two critical steps to obtaining useful information from tomography i) the reconstruction of a 3D image from 2D projections and ii) the analysis and quantification of features in the 3d object. While the techniques is rapidly growing in popularity, most users have fairly limited options when trying to recover the 3D image and are able to write only fairly primitive computer programs to extract key features from the images. The aim of this Collaborative Project is to establish a toolbox within which different reconstruction algorithms, artefact reduction codes, and image analysis procedures are made available to all.

[ICE – CSE, industry targeted software for future computer systems \(Hartree Centre\)](#)

Links to [CSED](#)

New centre with a need to establish joint projects and collaboration.

[Software engineering support programme \(SESP\)](#)

Links to [CCP NC](#), [CCP Forge](#)

The Software Engineering Support Programme (SESP) is an EPSRC support activity, funded through the SLA, to provide and encourage the use of up-to-date software engineering techniques and tools in software development within computational science and engineering.

[CCP NC: NMR crystallography](#)

Links to [ASEArch](#), [CCP Forge](#), [CCPN](#), [dCSE](#)

CCP-NC supports a multidisciplinary community of NMR spectroscopists, crystallographers, materials modellers and application scientists by developing and integrating software across the area of NMR crystallography. This is an emerging field, defined as the combined use of experimental NMR and computation to provide new insight, with atomic resolutions, into structure, disorder and dynamics in the solid state.

[Software repository for CCPs \(CCPForge\)](#)

Links to [ASEArch](#), [CCP12](#), [UKCP](#), [CCP5](#), [SESP](#), [CCP9](#), [CCPi](#)

CCPForge is a collaborative software development environment tool for the Collaborative Computational Projects. The CCPForge project is funded by The Joint Information Systems Committee (JISC) and is maintained by the Computational Science and Engineering Department of the Science and Technology Facilities Council under the departmental SLA with EPSRC.

[ASEArch CCP](#)

Links to [CCP-BioSim](#), [CCPNC](#), [CCPi](#), [CCP12](#), [CCP5](#), [CCPQ](#), [CCP9](#), [CSED SLA](#), [CCP Forge](#), [NA network](#), [emerging software technology](#), [dCSE](#), [UKTC](#), [SSI](#), [greater scalability](#)

Algorithms and Software for Emerging Architectures (ASEArch) is an EPSRC-funded Collaborative Computational Project (CCP). Led by the Oxford e-Research Centre, in collaboration with STFC staff at both Daresbury and RAL, ASEArch will investigate the use of novel architectures such as NVIDIA GPUs, and

Intel's Many Integrated Core (MIC) accelerators.

ASEArch works with other CCPs to assess the suitability of new architectures for their applications, and where appropriate assist them in porting to these new platforms.

[CCP12: HPC for engineering](#)

Links to [ASEArch](#), [CCP Forge](#), [SLA](#), [UKTC](#), [HECToR CSE](#), [non equilibrium flow programme grant](#), [EESI](#), [UKAA](#), [Aeroacoustics consortium](#), [Flow consortium](#)

The scientific remit of CCP12 is to provide core support to the engineering community in the use of High Performance Computing. CCP12's vision and ambition is to ensure that UK researchers are able to tackle computational engineering grand challenges using the best available numerical methods and techniques and to accelerate the impact of UK computational engineering on national and international High Performance Computing facilities.

[Emerging Software Technology](#)

Links to [ASEArch](#), [NA network](#), [NAIS](#), [CCPQ](#), [SLA](#)

Research is being undertaken across disciplines to develop emerging software technologies that will tackle future software engineering challenges; examples include compilers for multi-core, many-core, GPU, FPGAs, domain specific languages and computational science application frameworks.

[EPSRC network on numerical Algorithms and high performance computing](#)

Links to [NAIS](#), [ASEArch](#), [emerging software technology](#), [GPU algorithms](#), [SLA](#)

The purpose of this network is to provide a focus for a new collaboration between numerical analysts, computer scientists and developers and users of software and HPC within the nodes, supported by the necessary administrative organization. In partnership with [NAIS](#), the network aims to build a new interdisciplinary community at the numerical algorithms/HPC interface and thereby provide added value to existing funded research at the nodes in numerical algorithms and in HPC and its applications.

[CCP5: Condensed phases](#)

[ASEArch](#), [HECToR](#), [HECToR CSE](#), [CCP-BioSim](#), [CCP Forge](#), [SLA](#)

CCP5 is the Collaborative Computational Project for computer simulation of condensed phases and is funded predominantly by EPSRC. It promotes the involvement of UK scientists in collaborative research in this area. This is achieved through a programme of one- and two- day workshops, through facilitating tours of the UK by internationally leading scientists and through a series of flagship projects designed to produce cutting-edge software for the benefit of the CCP5 community. CCP5 also runs an annual Summer School that instructs 60-70 graduate students in the art of statistical-mechanics based simulation methods.

[SLA between STFC and EPSRC](#)

Links to [ASEArch](#), [HECToR CSE](#), [Universities CSE](#), [dCSE](#), [non equilibrium flow programme grant](#), [CCP-BioSim](#), [CCPNC](#), [CCPi](#), [CCP12](#), [CCP5](#), [CCPQ](#), [CCP9](#), [MCC](#), [UKCP](#), [UKTC](#)

The Computational Science and Engineering Department (CSED) at Daresbury provides the EPSRC community with computational support through a variety of mechanisms. Currently the support is provided via a Service Level Agreement (SLA) between EPSRC and STFC which is of the order of £2.5 million a year.

[CCP-BioSim: Biomolecular simulation](#)

Links to [ASEArch](#), [SLA](#), [CCP5](#), [dCSE](#)

A collaborative computational project in biomolecular simulation at the life sciences interface. CCP-BioSim aims to be an inclusive wide-ranging project, bringing together chemists, physicists and chemical engineers as well as researchers from all branches of 'molecule-oriented' biochemistry and biology. The

aim is to involve experimentalists and computational specialists, sharing the belief that the best science can be done when theory and experiment are closely integrated. CCP-BioSim aims to identify methodological and computational challenges in the field, and to foster developments to meet these scientific challenges. Involvement of early career academics is also an important goal and CCP-BioSim will also provide a networking and collaboration framework.

[CCP9: Electronic structure](#)

Links to [dCSE](#), [HECToR CSE](#), [SLA](#), [ASEArch](#)

The field includes the study of metals, semiconductors, magnets, and superconductors from microscopic quantum mechanical calculations. The activities of CCP9 encompass such highly topical areas as magneto-electronics (GMR, CMR, spin-transistors), photonics, nano-technology, high-temperature superconductors, and novel wide band gap semiconductors (e.g. GaN, diamond films).

CCP9 provides a network which connects UK research groups in electronic structure, facilitates UK participation in the larger [European ΨkNetwork](#), and has through a series of flagship projects developed a number of cutting edge computational codes.

[dCSE for HECToR](#)

Links to [NAG](#), [HECToR](#), [CCP-BioSim](#), [CCPNC](#), [CCPi](#), [CCP12](#), [CCP5](#), [CCPQ](#), [CCP9](#), [SLA](#), [ASEArch](#)

The aim of distributed CSE (dCSE) support is to enable software development to increase code performance and/or utility on computing facilities, and hence deliver further science. With a distributed CSE award researchers will receive support to improve the capability of their code on HECToR. The aim of the award is to provide the researcher with funding to enable them to employ specialist help to:

- port their codes onto HECToR, in particular to work with new codes or to enable previously unsupported features in existing codes;
- improve the performance of their codes on HECToR;
- re-factor their codes to improve long-term maintainability;

take advantage of algorithmic improvements in the field of high-performance computing.

[Numerical Algorithms Group \(NAG\)](#)

Links to [HECToR CSE](#), [Universities CSE](#), [dCSE](#)

NAG applies its expertise in numerical engineering to delivering computational software and high performance computing services. NAG's product and services portfolio includes the NAG Library, available in multiple guises, the NAG Compiler, and NAG's specialist Consulting and HPC services.

NAG is contracted by EPSRC, NERC and BBSRC to provide computational support to researchers using HECToR. Recently EPSRC have run a pilot scheme where NAG have supported researchers using regional and university machines.

[HECToR CSE Support](#)

Links to [NAIS](#), [HECToR](#), [HPC-SIG](#), [MCC](#), [UKCP](#), [UKTC](#), [CCP-BioSim](#), [CCPNC](#), [CCPi](#), [CCP12](#), [CCP5](#), [CCPQ](#), [CCP9](#), [SLA](#), [ASEArch](#)

The CSE Service exists to help the user community to make the best use of the HECToR machine by providing training, web-based resources, and assistance with porting, optimisation and tuning of software.

[NAIS \(Science and innovation award\)](#)

Links to [CRESTA](#), [emerging software technology](#), [HPC Short Courses](#), [HECToR CSE](#)

A UK-based Science and Innovation Centre investigating the algorithms and software methodology underpinning high performance computing.

[HPC-SIG](#)

Links to [HECToR](#), [HECToR CSE](#), [Universities CSE](#), [NAIS](#)

The HPC Special Interest Group was formed in 2005 in response to the significant funding for University-level computing funded primarily by the SRIF-3 funding round. Members are drawn primarily from Computing Services in the Higher Education sector with representation from related organisations such as the National Grid Service and funding bodies. The main Terms of Reference are, briefly:

- To act as a lobby stressing the value of mid-range HPC provision
- To ensure that HPC provision and research methodologies are closely aligned, promoting the academic agenda in addition to system management and support
- To collect, disseminate and promote best practice in HPC provision, management and support
- To coordinate and publicise training opportunities in the areas of HPC system support and usage within the UK
- To act as a link between National HPC provision and local University/campus level provision
- To act as an outreach vehicle promoting the use of HPC across all academic sectors
- To facilitate communication between academic and industrial/commercial HPC providers/users
- To secure the role of HPC as a vital research service across all academic disciplines

To demonstrate the value of HPC facilities in higher education and to ensure that these facilities can be delivered with best possible value for money

[HECToR](#)

Links to [HPC Short Courses](#), [HECToR CSE](#), [NAG](#), [Universities CSE](#), [HPC-SIG](#), [SLA](#), [UKTC](#), [UKCP](#), [MCC](#)

HECToR is the UK's high-end computing resource, funded by the UK Research Councils. It is available for use by academia and industry in the UK and Europe.

HPC education and training

Links to [e-Infrastructure Leadership Council](#), [HPC Short Courses](#), [HECToR CSE](#), [NAG](#)

Training and education in HPC, computing and software is undertaken in undergraduate and postgraduate taught courses at individual universities and by training organisations.

[Training marketplace from EGI](#)

Links to [SSI](#)

The EGI (European Grid Initiative) Training Marketplace is a service to coordinate training across communities, projects and national teams. The new Training Marketplace enables trainers to advertise events, materials and resources, and researchers using EGI to locate, access and comment on training material, events and resources that meet their needs.

[HPC short courses \(software development training\)](#)

Links to [Universities CSE](#), [PRACE Advanced Training Course](#), [NAIS](#), [HPC education and training](#), [EUDAT](#)

The High Performance Computing - Short courses consortium (HPC-SC) have designed a programme short training courses to help both new and established researchers to make optimal use of High Performance Computing (HPC) — whether the resources are provided locally, nationally, or internationally.

Universities CSE support

Links to [HPC Short Courses](#), [SLA](#), [HPC-SIG](#), [HECToR](#), [tier 2](#), [DiRAC](#)

Front line embedded research support for academics in computing, people and skills.

[International Exascale Software Project \(IESP\)](#)

Links to [EESI](#), [PRACE](#)

The IESP goal is to empower ultrahigh resolution and data intensive science and engineering research through to the year 2020 by developing a plan for a common, high quality computational environment for

peta/exascale systems and for catalysing, coordinating, and sustaining the effort of the international open source software community to create that environment as quickly as possible.

[European exascale software initiative \(EESI\)](#)

Links to [PRACE](#), [IESP](#), [CRESTA](#)

The objective of this Support Action, co-funded by the European Commission is to build a European vision and roadmap to address the challenges of the new generation of massively parallel systems composed of millions of heterogeneous cores which will provide multi-Petaflop performances in the next few years and Exaflop performances in 2020.

[European Data Initiative \(EUDAT\)](#)

Links to [SSI](#), [HPC Short Courses](#)

The EUDAT project aims to contribute to the production of a Collaborative Data Infrastructure (CDI). The project's target is to provide a pan-European solution to the challenge of data proliferation in Europe's scientific and research communities.

[PRACE advanced training centre](#)

Link to [HPC Short Courses](#), [PRACE](#), [HPC education and training](#)

Six PRACE members' sites: Barcelona Supercomputing Centre (Spain), CINECA - Consorzio Interuniversitario (Italy), CSC - IT Centre for Science Ltd (Finland), EPCC at the University of Edinburgh (UK), Gauss Centre for Supercomputing (Germany) and Maison de la Simulation (France) are the first PRACE Advanced Training Centres.

[2020 science \(EPSRC C-Dip fellowship programme\)](#)

Links to [VPH](#)

2020 Science is a collaborative research programme between the University of Oxford, University College London, and Microsoft Research, Cambridge. The programme is focused on fostering the creation of a new generation of future scientific leaders. At the heart of the programme is the development and application of novel computational approaches, methods and tools to address some fundamental problems in natural science, and the scientific computing, scientific software development and software engineering that underpin the development of predictive models of complex, multi-scale biological systems.

[US/UK software collaboration](#)

Links to [SSI](#)

EPSRC and NSF have released a joint call to develop and devise new software infrastructure, tools and architectures to enable the advance of solutions to grand challenges in the physical sciences. This should involve the close co-operation of communities in both the software and physical sciences domains to define and address the research challenges.

[APOS – EU](#)

Links to [CRESTA](#), [PRACE](#)

APOS-EU is funded by the European Commission and is in collaboration with a peer project APOS-RU that is funded by the Ministry of Education and Science of the Russian Federation. The projects will target a representative suite of simulation codes from the strategically important application areas of seismic modelling, oil- and gas-reservoir simulation, computational fluid dynamics, fusion energy, and molecular dynamics. The expertise and technologies that are developed in the course of this project will form a basis on which the wider scientific community can build, with a view to tackling the challenges of the Exascale computing era.

[G8 HORCS: NU – FUSE, G8 exascale fusion software](#)

The G8 Research Councils Initiative on Multilateral Research Funding is a coordinated effort to support multilateral research partnerships. The programme aims to support excellent research on topics of global relevance which can best be tackled by a multinational approach. Funding should help researchers to cooperate in consortia consisting of partners from at least three of the participating countries.

The initiative is supported by the Natural Sciences and Engineering Research Council of Canada (NSERC), the French National Research Agency (ANR), the German Research Foundation (DFG), the Japan Society for the Promotion of Science (JSPS), the Russian Foundation for Basic Research (RFBR), the Research Councils of the United Kingdom (RCUK), and the U.S. National Science Foundation (NSF), referred to as the Funding Organisations.

[CRESTA Collaborative Research Exascale Systemware Tools Applications \(FP7\)](#)

Links to [APOS-EU](#), [PRACE](#), [EESI](#), [VPH](#)

CRESTA brings together four of Europe's leading supercomputing centres, with one of the world's major equipment vendors, two of Europe's leading programming tools providers and six application and problem owners to explore how the exaflop challenge can be met.

The project has two integrated strands: one focused on enabling a key set of co-design applications for exascale, the other focused on building and exploring appropriate systemware for exascale platforms.

[Virtual physiological human network of excellence \(EU\)](#)

Links to [CRESTA](#), [2020 Science](#)

The VPH NoE is a project which aims to help support and progress European research in biomedical modelling and simulation of the human body. This will improve the ability to predict, diagnose and treat disease, and have a dramatic impact on the future of healthcare, the pharmaceutical and medical device industries.

[Correlated Multielectron Dynamics in Intense Light Fields \(CORINF\)](#)

The acronym CORINF stands for Correlated Multielectron Dynamics in Intense Light Fields. CORINF is a Marie Curie Initial Training Network (ITN) funded by the European Commission's Seventh Framework Programme (FP7). ITNs are designed to offer opportunities for researchers in the early stages of their careers to develop their skills and expertise as part of an international research network. Early Stage Researchers (ESRs) will receive multidisciplinary training within the project framework, which will culminate in them being awarded PhDs from partner institutions.

[CCPN](#)

Links to [CCP NC](#), [CCP-BioSim](#), [CSED](#)

CCPN is a public non-profit project, funded by the BBSRC, which serves the macromolecular NMR community and provides:

- Meetings to determine and spread best practice in NMR
- The CCPN Data Model for macromolecular NMR and related areas
- The CcpNmr programs suite: Analysis, ChemBuild, FormatConverter and SpecView
- A means to integrate existing NMR software within a unified system

[CCP4](#)

Link to [CCP-BioSim](#), [CSED](#)

The Collaborative Computational Project Number 4 in Protein Crystallography was set up in 1979 to

support collaboration between researchers working on such software in the UK, and to assemble a comprehensive collection of software to satisfy the computational requirements of the relevant UK groups.

[CCPEM: Electron cryo-microscopy](#)

Link to , [CSED](#)

MRC funded Electron cryo-microscopy collaborative computational project

[Square Kilometre Array \(SKA\)](#)

Links to [Diamond](#)

The Square Kilometre Array is a global science and engineering project to build the world's largest radio telescope. The project is led by the SKA Organisation, a not-for-profit company with its headquarters in Manchester, UK.

[BBSRC tools and techniques \(for HPC software\)](#)

An annual call run by BBSRC for funding for pump priming the next generation of tools, technologies and resources that will be required by bioscience researchers in scientific areas within BBSRC's remit.

[TSB KTPs for multicore and parallel processing](#)

The Technology Strategy Board has provided funding to stimulate a partnership working approach through the KTP (Knowledge Transfer Partnership) Programme, both to develop and exploit parallel computing technology to ensure that UK industry, across all sectors, remains competitive in terms of computing speed.

[EPSRC software fellowships](#)

EPSRC are looking to appoint fellows who have some experience of using and developing software in their chosen field and are looking to widen the use and usability of this software in order to undertake high quality research in Engineering or Physical Sciences. It is hoped that innovative approaches to this development and collaboration nationally, internationally and across disciplines will be supported.

[DiRAC](#)

Links to [tier 2](#), [Universities CSE](#), [e-Research South](#)

DiRAC is the integrated supercomputing facility for theoretical modelling and HPC-based research in particle physics, astronomy and cosmology, areas in which the UK is world-leading. It is supported by STFC.

[PRACE – research infrastructure](#)

[IESP](#), [EESI](#), [CRESTA](#), [APOS-EU](#), [PRACE advanced training centre](#)

The mission of PRACE is to enable high impact scientific discovery and engineering research and development across all disciplines to enhance European competitiveness for the benefit of society.

PRACE seeks to realize this mission through world class computing and data management resources and services through a peer review process. With the broad participation of European governments and associated countries through representative organizations, a diversity of resources can be provided by PRACE, including expertise throughout Europe in effective use of the resources.

[Software Sustainability Institute \(SSI\)](#)

Links to [JISC](#), [ASEArch](#), [EUDAT](#), [Training marketplace](#)

The EPSRC-funded Software Sustainability Institute works with researchers to identify and shape the software considered to be important to research. They provide a range of free and paid-for services which ensure that software is maintained, made available to a wider user base and its potential for sustainability is maximised.

The Software sustainability institute runs initiatives such as [software carpentry \(software programming for researchers\)](#), [community champions for research \(SeIUCCR\)](#) and [consultancy and best practice for research software projects](#).

[e-Infrastructure Leadership Council](#)

Links to [HPC education and training](#)

The E-Infrastructure Leadership Council (ELC) was established by Government in March 2012 following recommendations from the Government commissioned report [A Strategic Vision for UK e-Infrastructure \(2011\)](#).

Acting as a national advisory body, the ELC makes recommendations to Government on all aspects of e-Infrastructure. It provides a forum where representatives of academe, industry, the charitable and public sectors can come together to exchange views and discuss the development of e-Infrastructure, both nationally and globally.

[CSED at Daresbury](#)

Links to [SLA](#), [CCPN](#), [CCP4](#), [CCP EM](#), [ICE-CSE](#), [CCPP](#)

The Computational Science and Engineering Department (CSED) is based at the STFC Science and Innovation Centre in Daresbury. The major output of the department is the development and application of powerful simulation codes, usually in collaboration with university research groups. Particular emphasis is placed on achieving very high performance; advancing the basic computational methods to tackle new scientific challenges on new generations of hardware.

[Thermal and reactive flow consortium](#)

Links to [CCP12](#), [HECToR CSE](#)

Thermal and reactive flows are cross-cutting fundamental disciplines that have found applications in technologies such as aerospace engineering, combustion engines for power generation and propulsion, geothermal energy, solar thermal energy, bioenergy, nanotechnology, chemical engineering and climate science.

[Whole Engine Computational Aeroacoustics Consortium](#)

Links to [CCP12](#), [HECToR CSE](#)

Access to the HECToR resource to study various aeroengine flows/systems to produce noise reductions. The areas considered include the engine inlet rotor/fan zones, the combustor, turbine and exhaust.

[UK Applied Aerodynamics Consortium \(UKAA\)](#)

Links to [CCP12](#), [HECToR CSE](#)

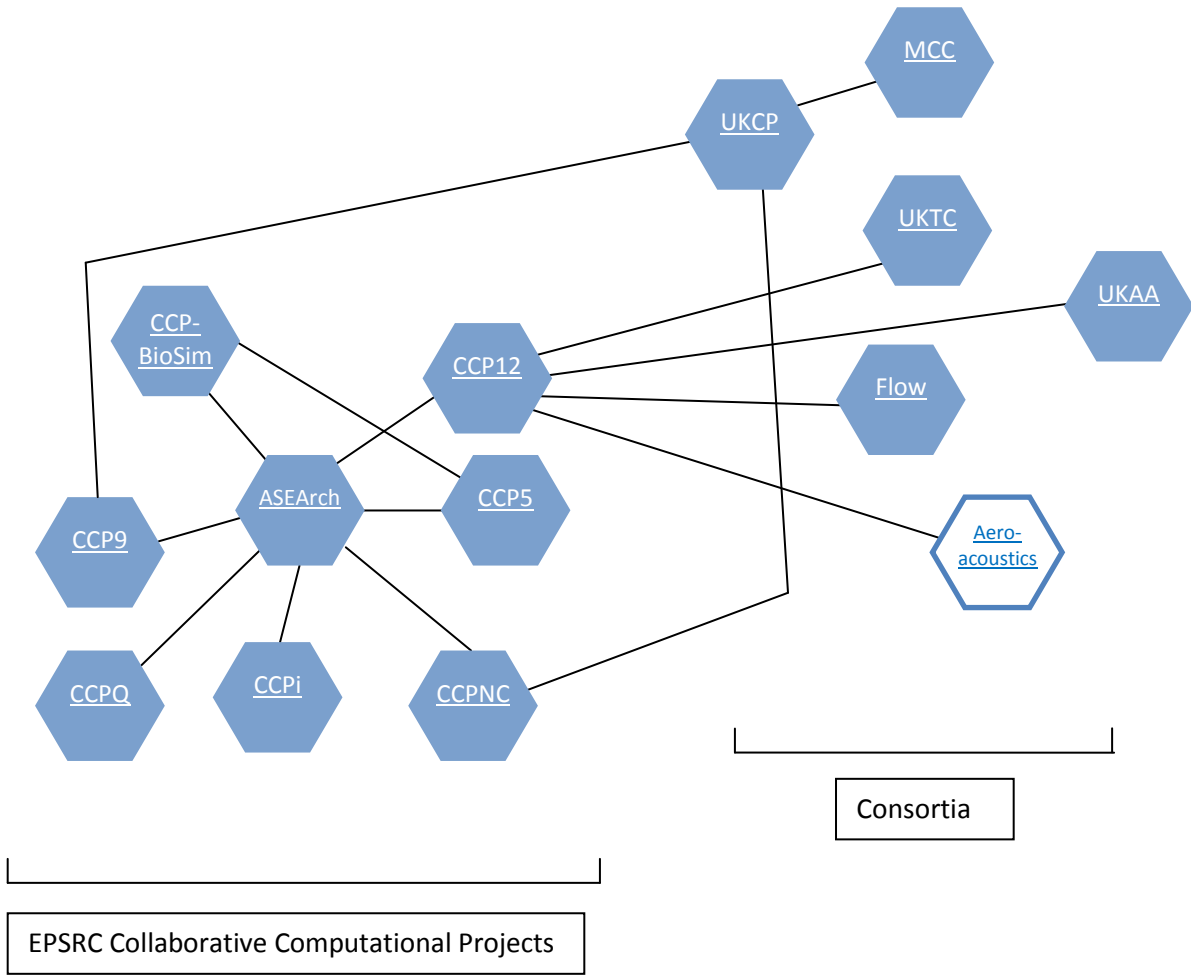
The UK Applied Aerodynamics Consortium provides for allocation units on the UK national supercomputers. Support for networking is also provided and is used to run consortium meetings and conferences. This consortium has been funded by EPSRC in the past but is currently not receiving direct support.

HPC software grants

EPSRC have funded a number of software-focussed grants through a variety of schemes. A selection of these grants is listed below.

- [Exploitation of High Performance Computing in the FLAME Agent-Based Simulation Framework](#)
- [Multi-scale simulation of intense laser plasma interactions](#)
- [Development of wide-ranging functionality in ONETEP](#)
- [HPC-GAP: High Performance Computational Algebra and Discrete Mathematics](#)
- [Wavepacket dynamics for the future: A general purpose HPC-compliant program](#)
- [Sustainable Software for Digital Music and Audio Research](#)





Annex 2: Forms

The forms from the afternoon session focussed on the following topics:

- 1: [Career Development](#)
- 2: [Co-ordination of Activities](#)
- 3: [Engagement and coordination with other funders \(incl. TSB\)](#)
- 4: [Training](#)
- 5: [Putting the middle into the pyramid](#)
- 6: [Widening Participation](#)
- 7a: [Preparing software for the next generation of computer systems](#)
- 7b: [Preparing software for the next generation of computer systems](#)

GROUP 1

Area: Career Development

Contributors

Ken Taylor (Champion), Ian Stewart, Tony Arber, David Quigley, Matt Farrow and Liping Zhao

Current Activities

1. Software development Fellowship (EPSRC)
2. Chartered engineers status
3. BCS (British computer society)
4. EPCC (have done something right to get to where they are. Supported by teaching).

Gaps

What are selection criteria for fellowships? – Papers vs. software

Who would be on the panel? – Developers should be

Recognition of S/W as research output

Are they targeting academic careers (or software developer careers)?

Recognition by HEIs, benefit of having software developers in senior posts

Tie in between training and career development.

Follow on for 5 year fellowships (what next – outputs not “REFable”)

Heading for software in ROS?

<i>What should be done and what would the outcome be?</i>	<i>How could this be achieved?</i>	<i>How much will it cost?</i>	<i>Benefits</i>	<i>EPSRC commentary post-workshop</i>
Ensure that software development fellowships are awarded to future research leaders in subject areas where computer science is vital to the subject.	Clarifying the selection criteria for fellowships. Speakers on panel need to be software developers as well as experts in applications. This also applies to the short-listing panel (even more importantly)	N/A	Renewal of research leadership in subject areas to which computer science is vital.	Application is the key driver for EPSRC's software fellowships and EPSRC would welcome computer science involvement. Research Infrastructure will work with colleagues in Physical Sciences and Engineering Themes to make sure that they are aware of the need for software development expertise to be covered by reviewers and panel.

Ensure that fellows are valued by their HEI at the end of the fellowship	Impact in REFs ROS Follow the cash – recognise the financial benefits of software development. Recognise long lead time of impact. Long term commitment to software development calls.		Savings in terms of efficient use of hardware/code re-use. Better productivity. Longevity of code	It is one of the aims of the fellowships that the importance of software development will be recognised by HEIs. Software development advances can be captured on the Research Outcome System .
Long term positions for software developers in HEIs and also Daresbury support role.	Accountability through identification of support through scientific entry on Je-S and EPSRC enforcing HEIs to let the money go that way.	Neutral	Continuity of knowledge	EPSRC will continue to support software development underpinning quality application science in the EPSRC remit, and those who provide it.
Develop linkage with computer scientists and developers to bring expertise and novel architectures into university groups and provide a career path at the support level within a university research group.	Funnelling 1 year internships into university groups	500k for 10 interns	Leverage from industry	Universities can already use the Doctoral Prize money which is part of their DTG allocation to undertake initiatives like this. Impact Acceleration Accounts, which are being awarded to 29 Universities, could also be used for this sort of support. Research Infrastructure will engage with EPSRC's Universities and Impact Teams and encourage conversations with senior University personnel about using these mechanisms to support software development activities.

GROUP 2

Area: Co-ordination of Activities

Contributors

Ian Reid (Champion), Nick Higham, Maxim Fedorov, Tom Jackson, Chris Greenough, Alun Ashton, Min Chen, Liping Zhao

Current Activities

1. Several support activities (e.g. RAL, NAG, Diamond, ISIS, CLF, Daresbury and European)
2. SSI – standardisation work and meta repository (working with Australia)
3. e-Leadership panel, HPC-SIG and Dave De Roure’s E-Infrastructure group - are they doing enough for users?
4. Active repository on cloud being developed at York – HEFCE Funded – now ready to roll.

Gaps

Bringing local activities together - sharing and transferring knowledge to prevent the wheel being re-invented.

Common repository for software – but how to judge quality on entries to know what work has already been done.

CSE support and users need to work in partnership.

<i>What should be done and what would the outcome be?</i>	<i>How could this be achieved?</i>	<i>How much will it cost?</i>	<i>Can something be achieved for half this?</i>	<i>EPSRC commentary post-workshop</i>
EPSRC funded meeting to bring local groups together for KT – EPS for CSE (reduce duplication of effort and share expertise)	Funded annual national meeting with preceding and trial software accessible. Encourage mixing of groups. 2-3 days, free to attend, open invitation, existing teams to take turns to organise.	£100k per meeting	Yes	An activity such as this could be coordinated through the Software Sustainability Institute. http://software.ac.uk/
Creation of UK repository for software (unless one already exists – we think not) (York Uni working on this – YouShare)	Possible existing resources. Encourage people to use. Looking for sustainable funding for YouShare. Investigate functionality of YouShare.	3 FTEs and Comp support. £1.5m/5 years	No (Might need more)	EPSRC are committed to providing funding to encourage sustainable software. We already support CCP Forge at RAL. We will investigate the requirements and what is available.

Software created with EPSRC funding should be made available to all UK researchers	EPSRC Policy	?	?	The Research Outcomes System encourages sharing of information. See above regarding code repositories.
Retaining expertise in the software development to maximise usefulness of software (link to career development group) (academics to value software developers more) -Train and re-train developers. -need more software engineers	Software development fellowships – encourage more of. Find out what CSE skills are available in community (e.g. taught course in CDT) and coordinate these resources.	?	?	We will keep the fellowships under review – demand, quality. Doctoral Prizes and Impact Acceleration Accounts can be used by universities to pursue some of these skills. EPSRC has been working with the HPC Short Courses Centre to link the activities to the existing CDTs.

GROUP 3

Area: Engagement and coordination with other funders (incl. TSB)

Contributors

Dave de Roure (Champion), Paul Caseley, Torsten Reimer, Adrian Wander, John Darlington, Nick Holliman, Fred Manby, David Chadwick, Juan Bicarregui

Current Activities

e-Leadership council - but what is their remit/TOR?
 EPSRC JISC funded projects
 TSB – digital strategy
 EPSRC digital social research
 RCUK DE theme

Gaps

X-RC funding for 'HPC' multidisciplinary projects
 Pull through for industry/Impact
 Other Govt departments (apart from BIS)
 TSB funding rules (50%-80%)

<i>What should be done and what would the outcome be?</i>	<i>How could this be achieved?</i>	<i>How much will it cost?</i>	<i>Can something be achieved for half this?</i>	<i>EPSRC commentary post-workshop</i>
Have a process for funding X-RC projects. No double jeopardy. Have RCUK road-map not individual RC's Explore links with other govt departments (home office, DoH, MOD).	Common budget line	?	?	There is an RCUK e-Infrastructure group which coordinates strategy across the RCs, and we will be developing a combined road-map. EPSRC has good links with TSB and NSF, with joint calls for software supported. The ELC will provide a forum for cross-government department discussions.
Re-integrate X-RC groups (tech watch) (incl. Industry and academia).				Research Infrastructure is currently restructuring its advice streams to simplify and incorporate all key stakeholders.
Find an issue to concentrate round (big data – volume, variety, variability) (shared technology issues – infrastructure).				This is covered in Groups 7A and 7B .

Funders to exchange info on their multidisciplinary activities	Have a meeting Have regular exchanges	?	?	EPSRC have regular meetings with their counterparts both at working level and at a strategic level to share information and discuss opportunities for collaboration.
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GROUP 4

Area: Training

Contributors

Mark Rodger (Champion), Adrian Mulholland, David Gavaghan, Alan Simpson, Claire Devereux

Current Activities

Courses through [HPC Short Courses](#), [SeIUCCR](#) and [SSI, 2020 Science](#)

Training embedded in CCPs and SLA

NAG/HECToR

Successful MSc project

PRACE programme

Universities individual post grad courses.

Gaps

1. Recognition that students need to develop software correctly – they don't realise!
2. Supervisors / research leaders need to be aware that software development is important.
3. Need better coordination between what already exists.
4. Transferable skills development.
5. Professional training – whether it be keeping in touch with what's going on or for cutting edge training.
6. Get them young before they go hacking!!
7. Coordination and awareness of the importance of computational science training.

Post-it comment – Supervisors are also ignorant/guilty. They don't realise the students are differently trained than they were.

<i>What should be done and what would the outcome be? How to incentivise culture change</i>	<i>How could this be achieved?</i>	<i>How much will it cost?</i>	<i>Can something be achieved for half this?</i>	<i>EPSRC commentary post-workshop</i>
<p>Could we have an EPSRC repository (e.g. modelled on Matlab central) for software dev.</p> <p>Central portal for IT- help people be aware of what is available.</p> <p>Then identify the gaps, plus any training that is required should be added to the database and made available for all.</p>	<p>Repository – make whatever is available clearly accessible.</p> <p>-video</p> <p>-lecture notes</p> <p>-within a VLE</p> <p>Need someone to manage it and collate material.</p> <p>Need some way to manage standards.</p>	<p>1 FTE and some machinery</p>	<p>On a shoestring – e.g. SSI might do it.</p>	<p>We intend to get training providers together to discuss what is available. We will explore at that meeting whether a central repository of training material would be welcome and feasible.</p> <p>We are also working with colleagues to ensure that the CDT call highlights the available training.</p>

Identify funds and location for regional development hubs (with industry and SME hubs)	Knowledge transfer to incentivise. Strategic call through EPSRC. Can we build on national HPC short courses? Could a CDT call include this? How to impact on regional training on software.	3 year champions post for computational science. Uni to match staff investment.	Fund half a post and see if will be matched by Uni. Fund half a post and make other half mandatory through CDT.	See above. The Software Sustainability Institute already has community champions who go to conferences and this initiative may be expanded.
Strategic opportunity through CDT call. CPD (funds for PhDs and ongoing career training).	Through CDT's but also need mechanism to train post docs	Normal / typical CDT cost	1 would be better than none.	See above. We will be encouraging CDT applicants to link in with the training that is already available.
Specialised and coordinated training for experts using cutting edge technology (e.g. exascale)	Possible through CDTs or other mechanisms. CDTs should be technique based - could use champion	?	?	There could be an opportunity to use the recently funded Tier-2 centres to pilot something in this area. The procurement for ARCHER also offers the opportunity to consider new approaches to training.
Encourage software skills into undergrad curriculum. Fund champions to put software skills into undergrad curriculum institution wide. Start debate with professional bodies "how do we embed computational science into a variety of disciplines?"	Start the debate to influence the curriculum. EPSRC should engage with: IoP, RSC, science minister, Royal college of eng, DoE, LMS, BIS, IMA, industry, syllabus boards, BCS. Graduate university involvement.	Almost cost free	?	Although undergrad teaching is outside of EPSRC's remit, we will continue to promote the importance of software skills at all levels with all our stakeholders.
Formulate a training centre on computational science for all applications.	Champions for undergraduate incorporation.	Time of local champions	To save money combine champions.	This is covered in comments above.

Find mechanism to incentivise.	Lower barriers and make material available. Career development for computational scientists. Force Universities to show how they collaborate.	?	?	See above.
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GROUP 5

Area: Putting the middle into the pyramid

Contributors

Anne Trefethen (Champion), David Chadwick, Peter Haynes, Robert Foster, Spencer Sherwin, Graham Riley, Tim Drysdale, Mark Basham, James Davenport, Milan Mihajlovic. John Darlington

Current activities

dCSE – HECToR, Universities.
Regional investments in computing facilities
University provision (growing)
Consortia – bringing in new users

Gaps

Policy
Scalable software
Consortia and regional clusters need to link
Appropriate resource allocation
Management of large data
Interface between science facility and home
Development environment
Funding of generic libraries?

Post-it comment – seems to assume that there is already a middle to the pyramid. It is important to note that - even after the December initiative - many Universities still don't have access to Tier-2 facilities. And those that were funded in December are sufficiently new initiatives that some thought needs to go into nurturing their survival (or even growth) beyond the next couple of years.

<i>What should be done and what would the outcome be?</i>	<i>How could this be achieved?</i>	<i>How much will it cost?</i>	<i>Can something be achieved for half this?</i>	<i>EPSRC commentary post-workshop</i>
Generic allocation unit across all facilities. Making sure there is appropriate use. Cost effective. Encourages people to join in.	EPSRC (RC) come up with AU definition. Accounting system coordinated.	Lots of people time	No	This makes sense, but it would be a challenge to get all the players together and agreeing. However, nonetheless it would be worthwhile exploring the feasibility with people.
De-bugging and profiling environment on many cores. More effective use of top of pyramid.	Enable interactive use on regional facilities. Set appropriate costs for interactive usage	Cost of licences (not cheap)	Yes – half as much	There needs to be consideration of the tools that are needed for software development and if there are further calls for tier 2 centres, consideration will be given to how this could be incorporated.

Link to widening and training. Scalable software up to medium/large. Develop flexible deployment software	CSE @ regional level? Transformative technology to enable scaling	Need to ask existing CSE and SSI (100k per year)	Yes – half as much	EPSRC has recently piloted funding dCSE support for universities and regional activities and this has received good feedback. This support could be continued or expanded and will be considered as part of the CSE procurement for ARCHER.
Enable regional and maybe cross regional support. More effective use of resource.	Over in careers group	?	?	This is covered in other comments.
Broadening remit of technical assessment (if doesn't need HECToR send elsewhere).	EPSRC policy	?	?	Again, this is a good idea. Links between the regional centres and the national resource need to be improved. The HECToR RAP Panel may provide a mechanism that we can adapt.
As first activity consortia and regional clusters need to link. Flexibility and opportunity and more options	Put requirement in next consortia call	?	?	This is covered in the comments above and the suggestion of new requirements if there is another consortia call is noted.
Hub for sharing technological developments (efficiency)	Physical network infrastructure (dark fibre). Infrastructure research council.	£££	possibly	Daresbury host the Machine Evaluation Workshop annually where vendors exhibit their latest technology and software developments. Other networking events may be appropriate here. EPSRC are hoping to support a mid-range facility in Dark Fibre . Any queries or comments on this should be addressed to Katie Blaney in the ICT team The E leadership Council has been established to bring different agencies together.

GROUP 6

Area: Widening Participation

Contributors

Neil Chue Hong (Champion), Jonathan Yates, Paul Sherwood, Catharine O’Sullivan, David Lecomber, Leigh Lapworth, Paul Caseley

Current Activities

People mobility
Sandpits
dCSE
CCP consortia renewal
Tier 2 regular clusters with industrial participation written in
Community champions
SSI Agents
CDTs

Gaps

Learned societies /Prof Orgs as broker, disseminator
Possible isolation of specialised SME
Infrastructure accessibility (between Unis)
Identifying pools of software expertise to tap into (and then how to tap into them)
Ease of use, reliable non-expert use
Not exploiting mechanisms to encourage under representative groups
Lack of computer scientists willing to apply – non cutting edge CS in projects (no incentive)

<i>What should be done and what would the outcome be?</i>	<i>How could this be achieved?</i>	<i>How much will it cost?</i>	<i>Can something be achieved for half this?</i>	<i>EPSRC commentary post-workshop</i>
Flexible IP arrangement for O-CSE	Review and modify IP arrangements (not one size fits all)	?	?	EPSRC makes no claims on the IP from the research it funds. This resides with the academic/university.
Software developer experts road shows with flexible pool of experts	Fund road shows and add resources to fund small collaborations made	£10k + £20k per grant	?	This is something we could explore with SSI.
Examine software engineering credentials of proposals	EPSRC enforcement and better guidance for proposers and reviewers. Review gates	?	?	Research Infrastructure is continually working with Themes across EPSRC to imbed best practice for software activities on proposals and will continue to do so. Stage gating of proposals was part of the last software development call and could be done in the future.

Support for ease of use, robustness, exploitation of software. (must show impact)	Wider consistency of beneficiaries	Equivalent to dCSE programme ? £1m +	?	This can be incorporated into the Pathways to Impact plan on all Research Council grants and associated funding can be requested. This is always highlighted in software calls, but we will explore whether it can be incorporated in the general guidance. Repositories could also be used to help here. See above.
Improve industrial participation / KT in CDTs	CDT-IPC	£6m	?	Priorities for CDT call are being developed, and industrial involvement will be a key element.
Increase awareness of industrial fellowships and KT secondments specific to software	Visiting professors (industry and academia) and distinguished scientists	£100k	?	These are already supported by EPSRC through a variety of mechanisms, but we will explore whether we can improve the publicity. We will also work with ELC to ensure these issues are addressed more widely.
Ensure calls are and feel open to those new to the area	Quota of new participants. Champions	£100k – £200k	?	We will continue to stress that the software strategy covers all aspects, not just HPC experts.
Bring together people from across disciplines	Sandpits, workshops	?	?	We agree this is a good idea; however, Research Infrastructure team is small and has limited time. We would be interested to hear from anyone willing to organise such events on our behalf.
Enable people to apply (non sexy) CS into projects/industry and be awarded	Change REF to be more open to having research outputs from other areas. Other measures of impact and research excellence are accepted by review panel	?	Make better use of industry, members of EPSRC college.	See above regarding the Research Outcome System.

GROUP 7A

Area: Preparing software for the next generation of computer systems

Contributors

Lorna Smith (Champion), Stephen McGough, Paul Kelly, Ross Nobes, Gerard Gorman, Sven –Bodo Schultz

Current activities

dCSE
 Software development grants
 POL open petascale libraries – Fujitsu
 Gung Ho
 CRESTA
 NAIS-Russia
 APOS-EU

Gaps

Communication / finding joint interest between computer scientists and application scientists.
 Still lack of funding for software re-engineering
 Preparedness of current codes for the disruptive future.
 Awareness of software engineering as important discipline.

<i>What should be done and what would the outcome be?</i>	<i>How could this be achieved?</i>	<i>How much will it cost?</i>	<i>Can something be achieved for half this?</i>	<i>EPSRC commentary post-workshop</i>
Support for interdisciplinary	Call. Different review process to solve the problem of people knowing half the proposal and ideas coming out of the blue.	3-5 years of significant funding (2-3 sites, 5 awards, £10m)	?	See new call. Applicants are encouraged to identify appropriate reviewers.
Matched funding for industrial projects. Good leverage, responsive mode. TSB. More welcoming RM. Put pressure on community to implement software best practice	Section reviewed separately – see Group 3			See joint call with TSB.

Changing the reviewing process. Specifically looking at science/software	SI2-US mech. Sub panel / changing culture. Software sustainability as part of proposal.	?	?	We have specifically asked for software management plans to be included in proposals to the new software call. We will assess the success of this, and whether this can be rolled out more widely.
Developing skills of application scientists to produce better code	Software carpentry (online?) How developing PHD in computational science + undergraduates	15k per event	?	See above.
Specific languages / higher level abstraction opportunities for disruptive tech	?	?	?	See new call.

GROUP 7B

Area: Preparing software for next generation computing

Contributors

Simon McIntosh-Smith (Champion), Rami Bahsoon, Adam Barker, Behzad Bordbar, James Cheney, Murray Cole, David Emerson, Adrian Jackson, Adrian Johnston, Richard Jones, Natalio Krasnogor, Matt Probert, Graham Riley, Ian Stewart, Mark van Schilfgaarde

Current Activities

Exascale – PRACE/CRESTA/EESI/FP7-EU
 Petascale – DCSE, NAIS, Gung-HO, HEA
 HPC S/W – S/W development call
 Regional HPC centres – Tier 2
 HEFCE modernisation fund – YouShare etc
 CCPS – ASEArch
 EPSRC/NSF Call
 BBSRC – Tools + techniques
 SSI – software sustainability
 SADEA call
 GU calls – CERES, ACELSR
 S/W fellowships

<i>What should be done and what would the outcome be?</i>	<i>How could this be achieved?</i>	<i>How much will it cost?</i>	<i>Can something be achieved for half this?</i>	<i>EPSRC commentary post-workshop</i>
Translational Gap from CS to Useful	Outcomes for science codes. Workshops Calls Matchmaking	£100k?	?	We agree this is a good idea; however, Research Infrastructure team is small and has limited time. We would be interested to hear from anyone willing to organise such events on our behalf. Also see new call.
EPSRC version of BBSRC tools and techniques	Projects	£100-£150k	?	These are essentially feasibility studies for software development. Both responsive mode and the new call offer opportunities.
Follow on? Existing is for commercialisation		£1-£1.5m	?	Funding for this already exists through the Doctoral Prizes and Impact Acceleration Accounts, as described in the commentary on Group 1 .

Tools/Libraries etc to make advanced architectures easier to use for domain scientists	Open SW EPSRC / JSC data / DCD standard call			See new call.
Big Data benchmarks	Join up producers and consumers			A networking activity may help here.
SW optimisation via machine learning et al and autotuning	EPSRC/RCUK + e.g. BBSRC, NERC ideas factory/call			See new call.
S/W that can address energy efficiency	Energy aware software. Fault tolerance. Massive scale,... repeatability			See new call, and joint call with TSB.
Repository	Grand challenge Identify key S/W components. Programme grant, networks,			See above – more work needed.
UK national computational science symposium	Part of MEW (machine evaluation workshop)			This could be incorporated into the Machine Evaluation workshop. It needs to be clear that this should be an EPSRC-funded activity and not one that should be managed by others.

Annex 3: Attendees

Surname	Forename	Institution	Activity
Arber	Tony	University of Warwick	Afternoon attendee
Ashton	Alun	Diamond Light Source	Afternoon attendee
Bahsoon	Rami	University of Birmingham	Afternoon attendee
Barker	Adam	University of St Andrews	Afternoon attendee
Basham	Mark	Diamond Light Source	CCP Tomographic Imaging
Bicarregui	Juan	RAL	Software support for facilities
Bordbar	Behzad	University of Birmingham	Afternoon attendee
Caseley	Paul	DSTL	Afternoon attendee
Catlow	Richard	UCL	Materials Chemistry consortium
Chadwick	David	University of Kent	Afternoon attendee
Chen	Min	University of Oxford	Afternoon attendee
Cheney	James	University of Edinburgh	Afternoon attendee
Chue Hong	Neil	University of Edinburgh	SSI
Cole	Murray	University of Edinburgh	S & I Award
Darlington	John	Imperial College London	Afternoon attendee
Davenport	James	University of Bath	Afternoon attendee
De Roure	Dave	University of Oxford	e-Science
Devereux	Claire	RAL	Crossing the Chasm
Drysdale	Tim	University of Glasgow	Afternoon attendee
Emerson	David	Daresbury	CCP12
Fedorov	Maxim	University of Strathclyde	Afternoon attendee
Foster	Robert	Queen Mary University	Afternoon attendee
Frangi	Alejandro	University of Sheffield	Afternoon attendee
Gavaghan	David	University of Oxford	LSI CDT
Gorman	Gerard	Imperial College London	Afternoon attendee
Greenough	Chris	RAL	CCP Forge
Haynes	Peter	Imperial College London	Afternoon attendee
Higham	Nick	The University of Manchester	Network – numerical algorithms
Holliman	Nick	Durham University	Afternoon attendee
Jackson	Adrian	University of Edinburgh	Afternoon attendee
Jackson	Tom	University of York	Afternoon attendee
Johnston	Adrian	Royal Holloway	Afternoon attendee
Jones	Richard	University of Kent	Jikes RVM
Kelly	Paul	Imperial College, London	ICT many Core w/s
Krasnogor	Natalio	University of Nottingham	Afternoon attendee
Lapworth	Leigh	Rolls-Royce plc	Afternoon attendee
Lecomber	David	Allinea Software	Afternoon attendee
Manby	Fred	University of Bristol	Afternoon attendee
McGough	Stephen	Newcastle University	Afternoon attendee
McIntosh-Smith	Simon	University of Bristol	ARCHER
Mihajlovic	Milan	The University of Manchester	Afternoon attendee
Mulholland	Adrian	University of Bristol	CCP-BioSim
Nobes	Ross	Fujitsu Labs of Europe	Afternoon attendee
O'Sullivan	Catherine	Imperial College London	Afternoon attendee
Probert	Matt	York University	Car-Parrinello consortium
Quigley	David	University of Warwick	CCP5

Reid	Ian	NAG	dCSE
Reimer	Torsten	JISC	Cloud
Riley	Graham	The University of Manchester	Afternoon attendee
Rodger	Mark	University of Warwick	Short courses
Scholz	Sven-Bodo	Heriot Watt University	Afternoon attendee
Sherwin	Spencer	Imperial College London	Chem s/w MRF
Sherwood	Paul	Daresbury	HEC
Simpson	Alan	University of Edinburgh	HECToR
Smith	Lorna	University of Edinburgh	PRACE
Stewart	Ian	University of Bristol	HPC-SIG
Taylor	Ken	QUB	CCPQ
Trefethen	Anne	University of Oxford	ASEArch CCP
van Schilfgaarde	Mark	King's College London	Afternoon attendee
Wander	Adrian	Daresbury	SLA
Yates	Jonathan	University of Oxford	CCP NMR
Zhao	Liping	The University of Manchester	Afternoon attendee