The UK's HPC Landscape and the HEC-WSI CoSeC Workplan

HEC-WSI
a High End Computing Consortium for Wave Structure Interaction

Stephen Longshaw,
UKRI STFC
Daresbury Laboratory

CoSeC
Computational Science Centre for Research Communities

Introduction to STFC

HM Government

Department for Science, Innovation & Technology

UK Research and Innovation

Science and Technology Facilities Council

Scientific Computing

Arts and Humanities Research Council
AHRC funds outstanding original research across the whole range of the arts and humanities.

Biotechnology and Biological Sciences Research Council
BBSRC invests to push back the frontiers of biology and deliver a healthy, prosperous and sustainable future.

Economic and Social Research Council
ESRC is the UK's largest funder of economic, social, behavioural and human data science.

Engineering and Physical Sciences Research Council
EPSRC creates knowledge in engineering and physical sciences for UK capability to benefit society and the economy.

Innovate UK
Innovate UK is the UK's national innovation agency supporting business-led innovation in all sectors, technologies and UK regions.

Medical Research Council
MRC funds research at the forefront of science to prevent illness, develop therapies and improve human health.

Natural Environment Research Council
NERC is the driving force of investment in environmental science.

Research England
Research England funds and engages with English higher education providers, to create and sustain the conditions for a healthy and dynamic research and knowledge exchange system in the higher education sector.

Science and Technology Facilities Council
STFC supports research in astronomy, physics, space science and operates world-class research facilities for the UK.

What are <u>H</u>igh-<u>e</u>nd <u>C</u>omputing Consortia?

- The HECs are four-year EPSRC funded projects.

- They provide their members and users with access to computing resources on the national HPC services like ARCHER2, enabling research in areas of science or engineering.

- The HEC concept can be traced back to the early 1990s where a need for organised consortia to utilise national supercomputing facilities became evident as part of the wider UKRI funded Collaborative Computational project (CCP) activities.

- There are currently 6 HECs around different scientific areas.

- The HECs are supported by STFC's **Co**mputational **S**cience C**e**ntre for Research **C**ommunities (CoSeC).

https://www.archer2.ac.uk

What is CoSeC?

- A cross-council funded programme run by STFC Scientific Computing

- Working with: council funded collaborative consortia

- On aspects of computational science around:
  - Scientific software - development, support & maintenance
  - Collaborative and fundamental research
  - Training and outreach
  - Development of methods and techniques
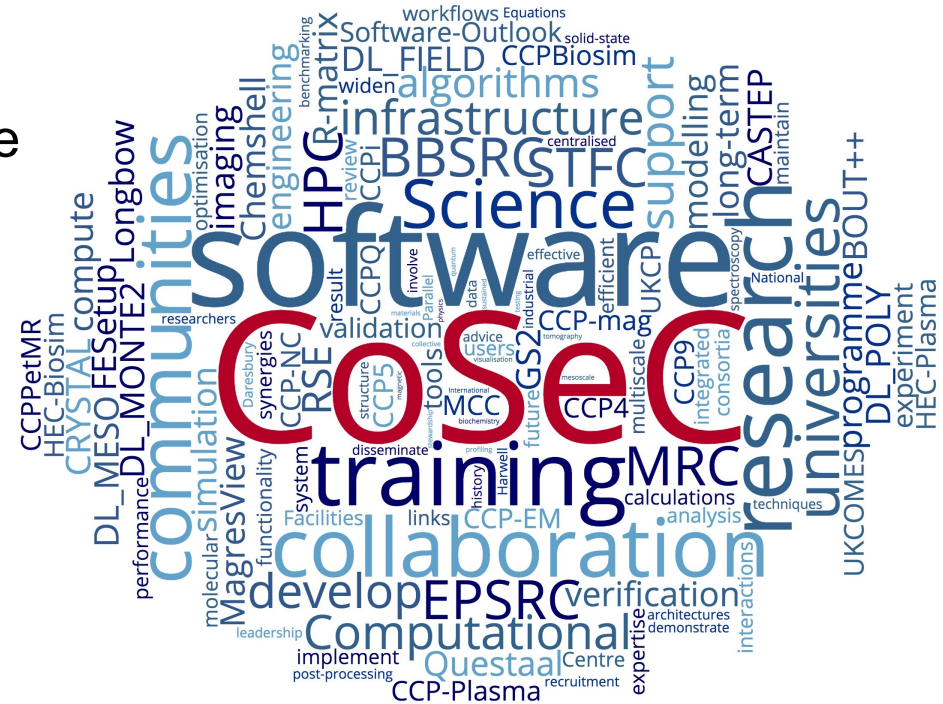
What areas of science does CoSeC work in?

- CoSeC is:
  - Around 60 STFC Computational Scientists, Research Software Engineers and support
  - Support for the Collaborative Computational Projects (CCPs) and High-end Consortia (HECs)
- CoSeC's science is shaped by the CCP and HEC landscape:
  - Materials Science
  - Tomographic Imaging
  - Computational Engineering
  - Biological Science
  - Quantum computing
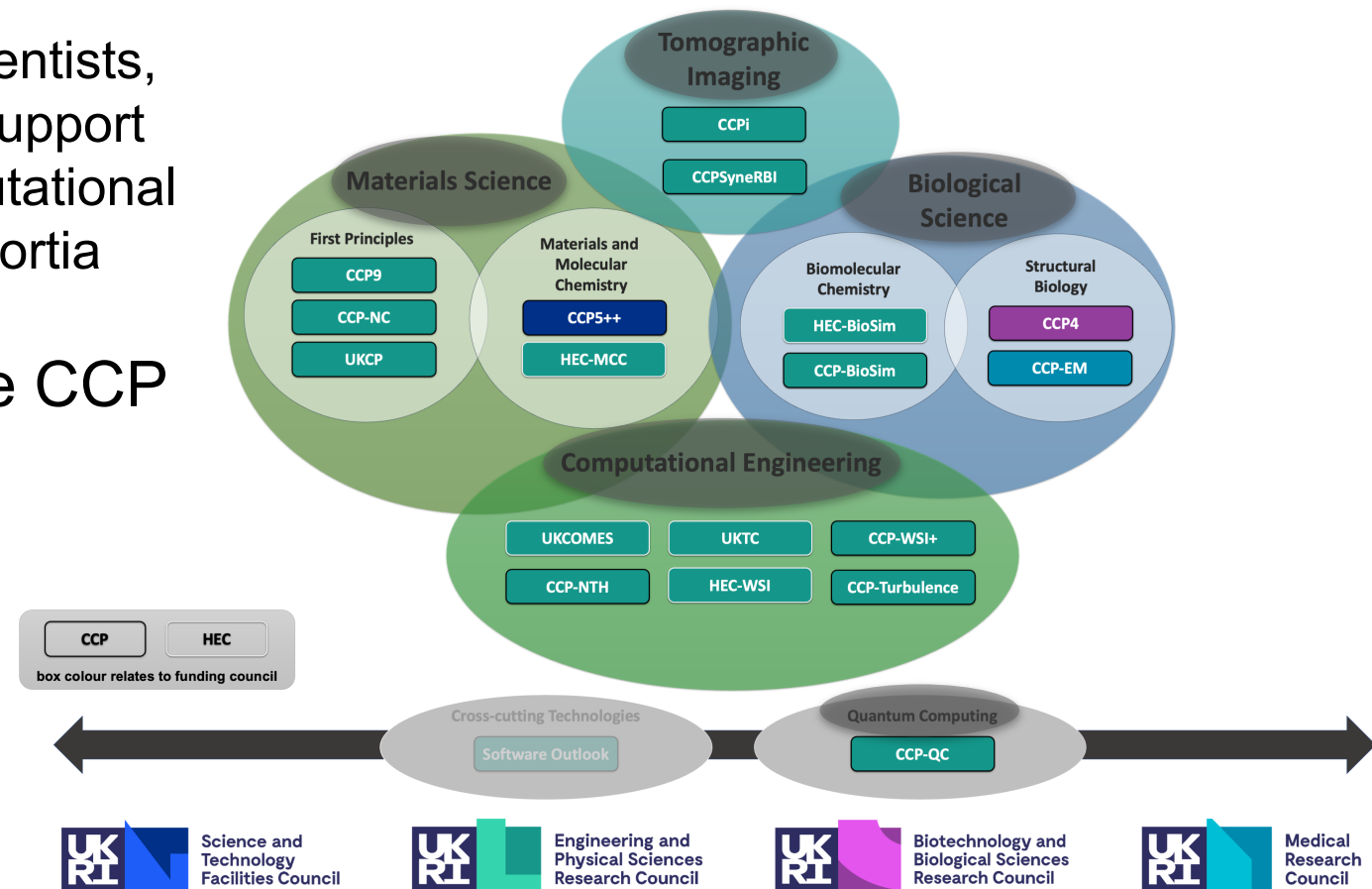
The UK HPC Landscape

High-Performance Computing (HPC) in the UK

- To date, HPC (or Supercomputing) in the UK has been driven by individual research councils (e.g. EPSRC, NERC & STFC)
  - ARCHER2
  - DiRAC
  - Bede (N8)
  - Cirrus
  - … many others
  - https://www.hpc-uk.ac.uk/
- These are split into Tiers:
  1. National (**ARCHER2**, DiRAC)
  2. HPC centre (Cirrus, Bede)
  3. Local (your favourite local cluster)

High-Performance Computing (HPC) in the UK

- The creation of UKRI in 2018 offered the chance for a new approach
- The UKRI wide Digital Research Infrastructure (DRI) strategy was created

- Potential upsides:
    - Larger pots of money to create internationally significant HPC resources
    - Enhanced collaboration to find more widely applicable approaches

- Potential downsides:
    - Loss of domain-specific optimisation
    - Reduction in scope and variety of national infrastructure if council-led efforts reduce as a result

https://www.ukri.org/what-we-do/creating-world-class-research-and-innovation-infrastructure/digital-research-infrastructure

High-Performance Computing (HPC) in the UK

- The actual reality of UKRI DRI is still unfolding:
  - A £900 million investment into a new national AI computing resource and a new **exascale** supercomputer was announced by the chancellor in the 2023 spring budget.
  - Part of the AI resource was announced recently as the **Isambard-AI** service hosted by Bristol University at the National Composites Centre (NCC).
  - It has been announced that the Edinburgh Parallel Computing Centre (EPCC) who host ARCHER2 will also host the new exascale system, with work starting in 2025.
- Key questions are:
  - Is the UK now creating a new Tier-0 for national UKRI DRI HPC infrastructure?
  - What happens to the current Tier-1 (i.e. ARCHER2) – does this become the new exascale system or will EPCC host both
  - What will the Isambard-AI and exascale systems look like in terms of architecture?

Science and Technology Facilities Council

Scientific Computing

Exascale?

- What is exascale?
- Simply put, a single supercomputer capable of calculating 10^{18} floating point operations per second (over 40x that of ARCHER2)
- According to the official TOP500 list of supercomputers in the world (https://www.top500.org) there is officially one of these systems in the world:
  - Frontier at Oak Ridge National Laboratory in the USA
- Others are likely exist in China
- The EU recently announced JUPITER as part of the EuroHPC programme which will be hosted at the Jülich Supercomputing Centre.
- Japan is also working on its next big system Fugaku-NEXT

Exascale?

- All exascale systems so far (both Frontier and those announced) have been *heterogeneous* in their design – a mixture of CPUs and accelerators (GPUs)
- No current reason to expect the UK's system to be different
- This is fundamental to HPC communities like HEC-WSI

The future of HPC is not a homogeneous system like ARCHER2, it is a heterogeneous system where you <u>have</u> to make efficient use of huge numbers of different types of interconnected processor

Scientific Computing

The Path to Exascale?

- The UK has been investing in the UKRI DRI path to exascale:
  - The 5 year £50m **Ex**ascale **C**omputing **AL**gorithms & **I**nfrastructures **B**enefiting **U**K **R**esearch (ExCALIBUR) programme
  - Investment into existing UK HPC to provide "pre-exascale" platforms
  - Long-term investment into the High-end Computing Consortia and programmes like CoSeC
- Investments also made through the EuroHPC and the Horizon funding programmes like the exaFOAM project
- However… exascale is a reality, it will be with us in the UK within the next 2-4 years and before that, use of HPC far larger than ARCHER2 is likely to be available.

Communities like HEC-WSI need to leverage ARCHER2 right now to be able to move onto what is coming next, the HEC is a great resource to get started

https://exafoam.eu   **https://excalibur.ac.uk**

The HEC-WSI CoSeC Workplan

Scientific Computing

What is CoSeC doing in HEC-WSI?

1. Providing computational science support to the entire community:
   - Scientific software development
   - Algorithmic developments
   - HPC application performance engineering
   - Training
2. Helping enable computational infrastructure (e.g. website, data collation)
3. Undertaking a specific workplan within the project itself

Science and Technology Facilities Council

Scientific Computing

The CoSeC Workplan

- This plan is **flexible** – it is a starting point but can (and should) change according to the communities needs

- Key work packages:

  - **Porting, optimisation and code developments for WSI**
    - *Looking at key codes like OpenFOAM, ParaFEM, FEniCS and performing WSI-specific profiling on ARCHER2, looking at developments in GPU acceleration and sharing best practices and directly optimising WSI community codes.*

  - **Scientific use case development and sharing**
    - *Working directly with a dedicated Research Software Engineer (RSE) at Plymouth University, helping to develop use cases to demonstrate WSI HPC need and capability.*

  - **Training and dissemination**
    - *Development and support of infrastructure to help distribute access to ARCHER2 and providing training around topics like code development and HPC use.*

UKRI
Science and Technology Facilities Council

Scientific Computing

Conclusions

- CoSeC is a long-standing programme run by STFC and designed to provide computational science support to communities like the CCPs and HECs.
- Fundamentally HECs like HEC-WSI are here to enable the use of national computing resources like ARCHER2 by providing computational access as well as scientific software support.
- The nature of HPC in the UK is changing, both in terms of scope and scale.
- The future of HPC is heterogeneous, large-scale parallelism – large numbers of CPUs connected to hugely powerful GPUs.
- CoSeC works directly within HEC-WSI and is available to provide computational science support to its community as well as undertaking a specific plan within the project.

Science and Technology Facilities Council

Scientific Computing

Questions?

Annual Conference 2023
Wednesday 6 December @ CIUK 2023

www.scd.stfc.ac.uk/Pages/CoSeC-Conference-2023.aspx