The Computational Science Centre for Research Communities

Stephen Longshaw,
Damian Jones (PM),
Mai Hoang (admin),
Alison Oliver (communities & impact),
Pankaj Pathania (finance),
Georgia Lomas (events)

Enables computational research by developing software **as an infrastructure** to address complex problems requiring advanced computing

A UKRI funded Centre to deliver, enable and support collaborative computational research

Achieved through **stable long-term holistic partnerships** with researchers organised as UKRI-funded communities

CoSeC

STFC Scientific Computing

- A department within STFC's National Laboratories
- Provides direct computational infrastructure, science and engineering support to STFC's national facilities and users
- Also working externally with researchers across UKRI and internationally
- 300+ Research Technical Professionals (RTPs) based at both STFC's Daresbury and Rutherford Appleton Laboratories
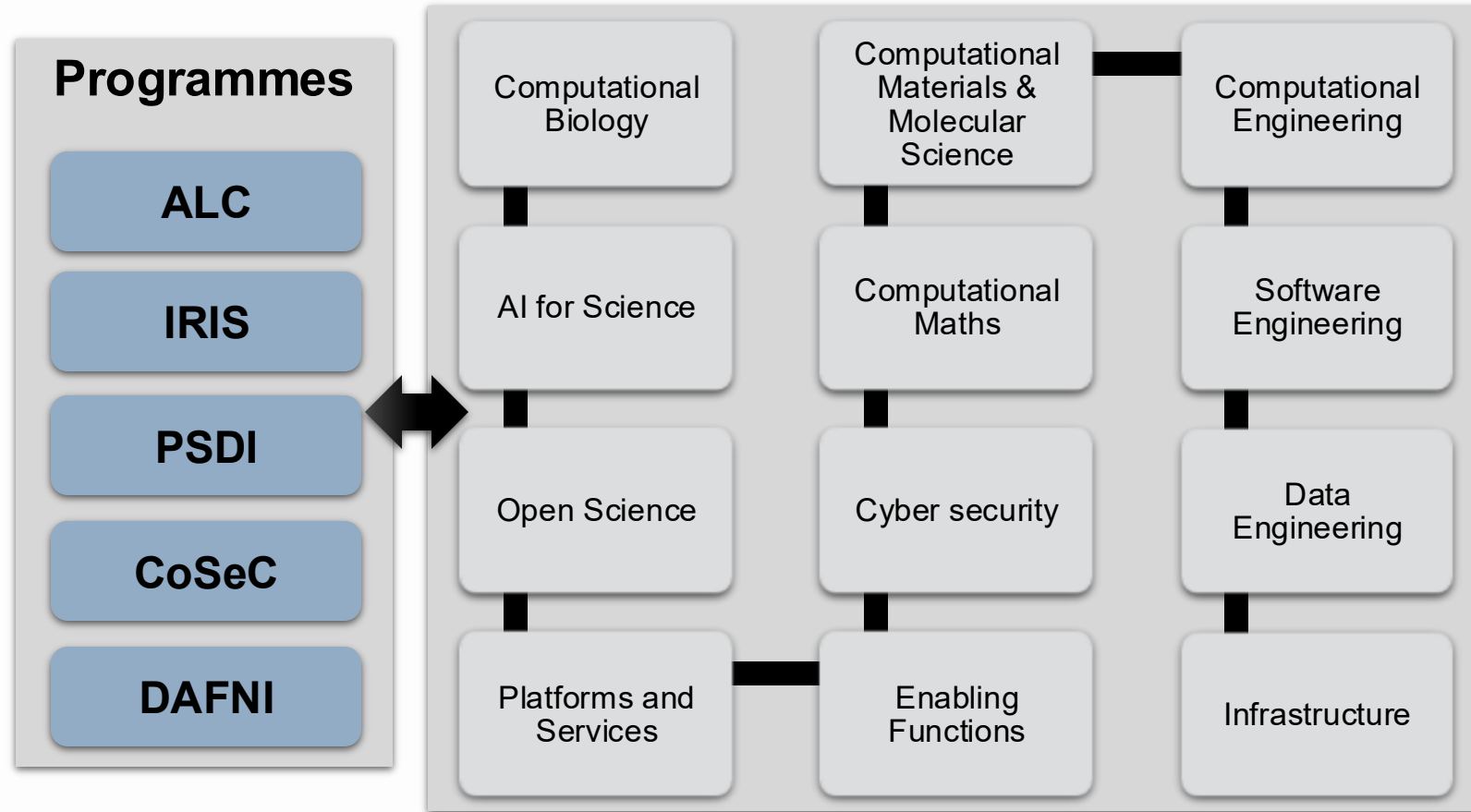

Daresbury Laboratory
Warrington, Cheshire

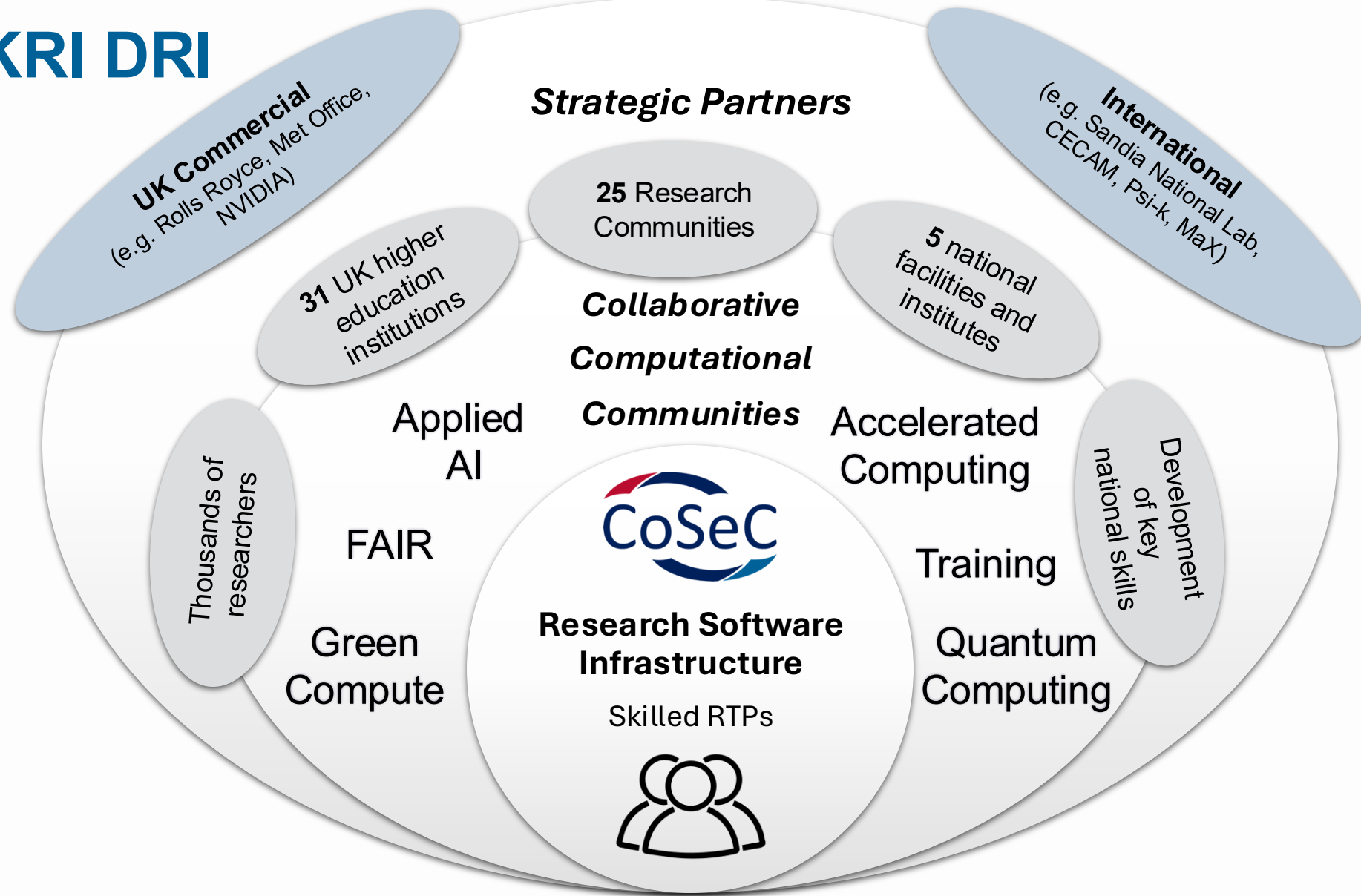Rutherford Appleton Laboratory
Chilton, Oxfordshire

CoSeC is part of STFC Scientific Computing

CoSeC is designed as a programme and cuts across the department's themes, drawing from their staffing, skills, co-ordination and leadership.

Programmes			
ALC	Computational Biology	Computational Materials & Molecular Science	Computational Engineering
IRIS	AI for Science	Computational Maths	Software Engineering
PSDI	Open Science	Cyber security	Data Engineering
CoSeC	Platforms and Services	Enabling Functions	Infrastructure
DAFNI			

A Part of the UKRI DRI

- ✓ Sharing of expertise
- ✓ Shared aims and strategy
- ✓ Community driven research software development
- ✓ Shared approaches to data
- ✓ **Greater value from research**

Strategic Partners

UK Commercial (e.g. Rolls Royce, Met Office, NVIDIA)

International (e.g. Sandia National Lab, CECAM, Psi-k, MaX)

25 Research Communities

31 UK higher education institutions

5 national facilities and institutes

Collaborative Computational Communities

Thousands of researchers

Applied AI

FAIR

Green Compute

Accelerated Computing

Development of key national skills

Training

Quantum Computing

CoSeC

Research Software Infrastructure

Skilled RTPs

Core CoSeC Team

Stephen Longshaw
Director

Mai Hoang
Administrator

Damian Jones
Programme Manager

Georgia Lomas
Events Manager

Alison Oliver
Research Communities Manager

Cross-cutting

Gemma Poulter
Research Object Cataloguing

Jessica Huntley
Sustainable Software

New Communities

James Gebbie-Rayet
CCPBioSim,
HECBioSim, CCPN

Wei Wang
CCP-NTH

Eugene Krissinel
CCP4

Kane Shenton
CCP-NC

Evgueni Ovtchinnikov
CCPSyneRBI

Alin Elena
CCP5, CCP-QC

Wendi Liu
CCP-WSI, HEC-WSI

David Emerson
UKNR

Valantis Tsinginos
CCC-ParaSolS

Alastair Dewhurst
CCP-TEPP

Stefano Rolfo
CCP Turbulence,
UKTC

Edoardo Pasca
CCPi

Tom Burnley
CCP-EM

Dominik Jochym
UKCP

Michael Seaton
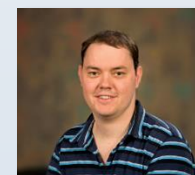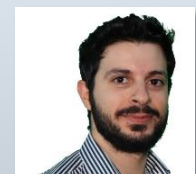UKCOMES

Thomas Keal
HEC-MCC

Leon Petit
CCP9

Jeyan Thiyagalingam
CCP-AHC

Hussam Al Daas
CCP-DCM
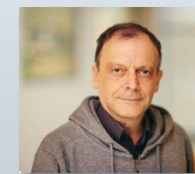
Martyn Winn
CCP-VEM

CoSeC

CoSeC in 2024

- £4.5m in community funding through STFC, alongside direct and ongoing technical support from CoSeC's Research Technical Professionals (RTPs) within the communities

- Thousands of *technical training days* delivered by CoSeC RTPs with the communities

- A new cohort of CoSeC Fellows – providing funding for each to be a CoSeC ambassador

- Town Hall event in July that brought researchers together from across UKRI to discuss collaborative computational research

- Platforms for computational researchers through the CoSeC impact award and conference

2024 CoSeC Conference
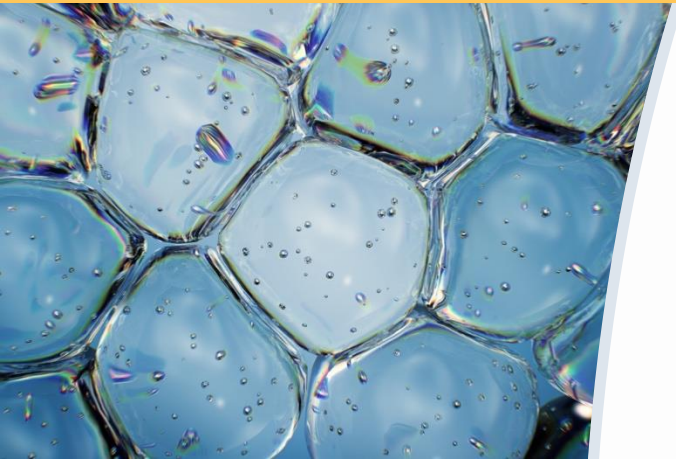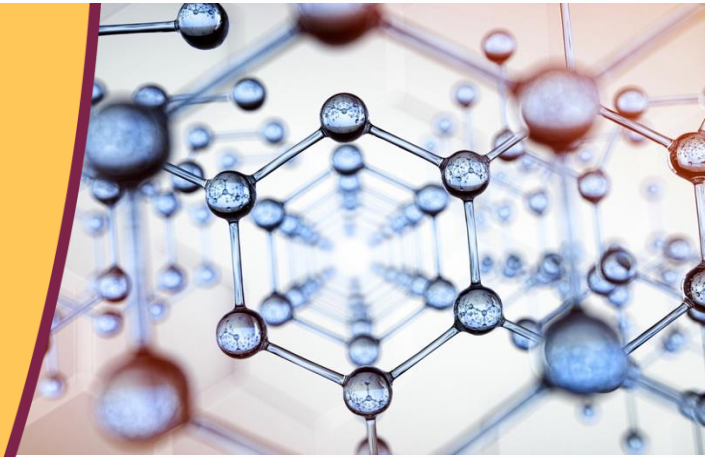December 2024 – CIUK, Manchester

CoSeC Town Hall
July 2024 - Manchester

CoSeC Impact Award Winner
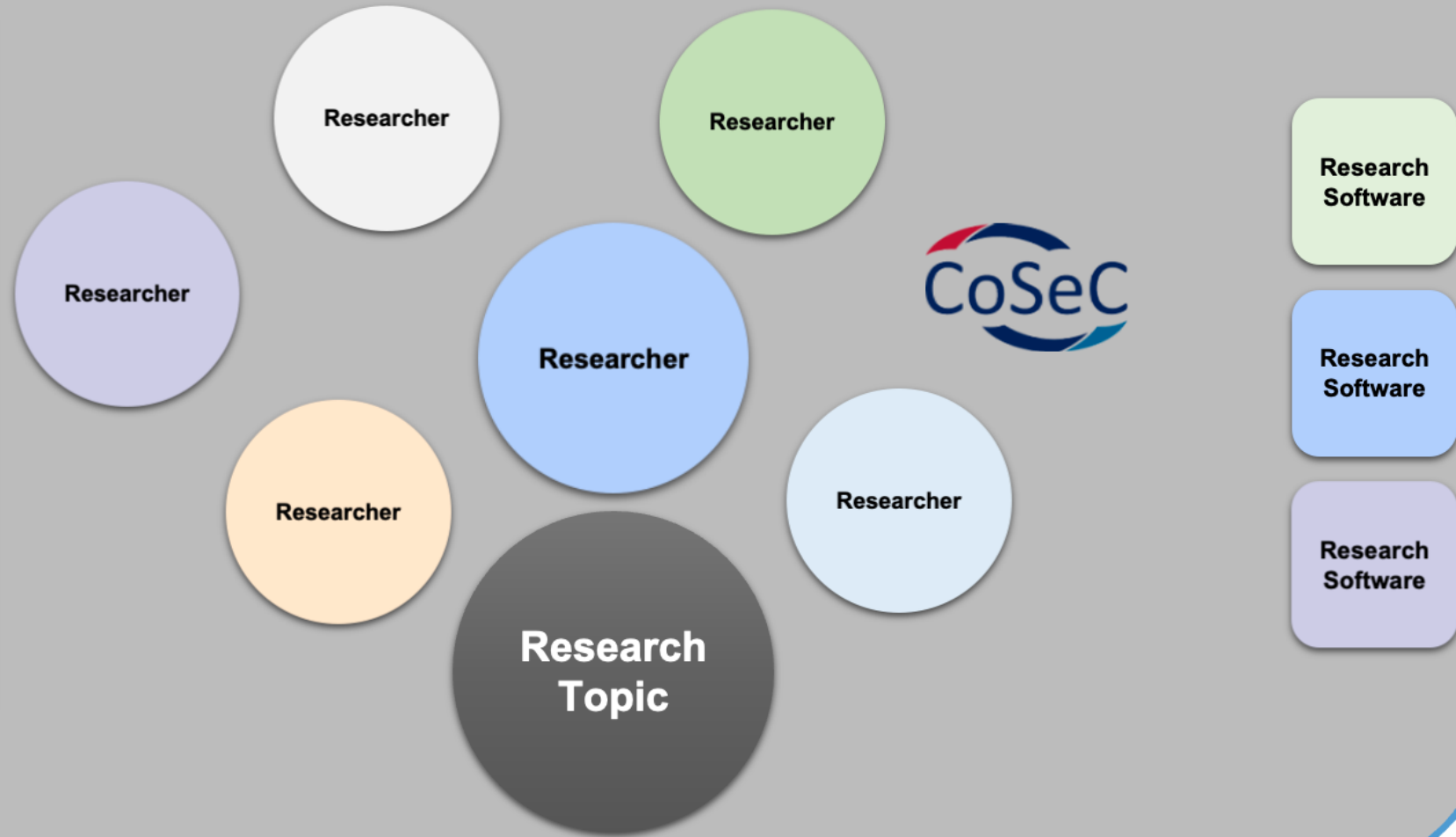Dr Thomas Zillhardt (CCPi)

Collaborative Computational Communities

Collaborative Community Model

- ✓ Sharing of expertise
- ✓ Shared aims and strategy
- ✓ Community driven research software development and maintenance
- ✓ Shared approaches to data
- ✓ **Greater value from research software**

Community Landscape

- CoSeC directly funds and supports 13 CCPs and 6 EPSRC funded HECs
- From 2025 CoSeC funds and supports 6 scoping projects to develop new communities

Materials

- **CCP9**: Electronic Structure of Condensed Matter
- **CCP-NC**: NMR Crystallography
- **CCP5**: Simulation of Condensed Phases
- **UKCP**: Car-Parrinello Quantum Mechanics (HEC)
- **MCC**: Material Chemistry (HEC)

Biology

- **CCP4**: Protein Crystallography
- **CCP-EM**: Electron Cryo-microscopy
- **CCP-N**: NMR Spectroscopy
- **CCPBioSim**: Biomolecular Simulation
- **HECBioSim**: HPC within Biomolecular Simulation (HEC)
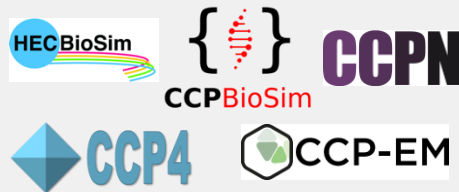
Imaging

- **CCPi**: Tomographic Imaging
- **CCPSyneRBI**: Synergistic Reconstruction for Biomedical Imaging

Engineering

- **CCP-WSI**: Wave Structure Interaction
- **CCP-NTH**: Nuclear Thermal Hydraulics
- **CCP-Turbulence**: Complex Turbulence modelling
- **UKTC**: HPC for Turbulence modelling (HEC)
- **UKCOMES**: Mesoscale Engineering (HEC)
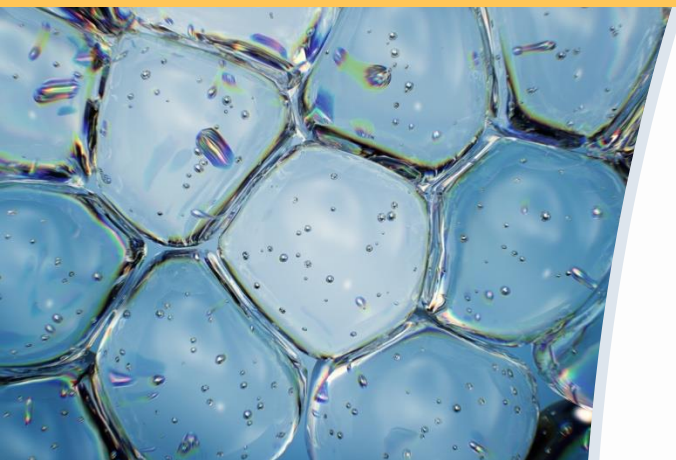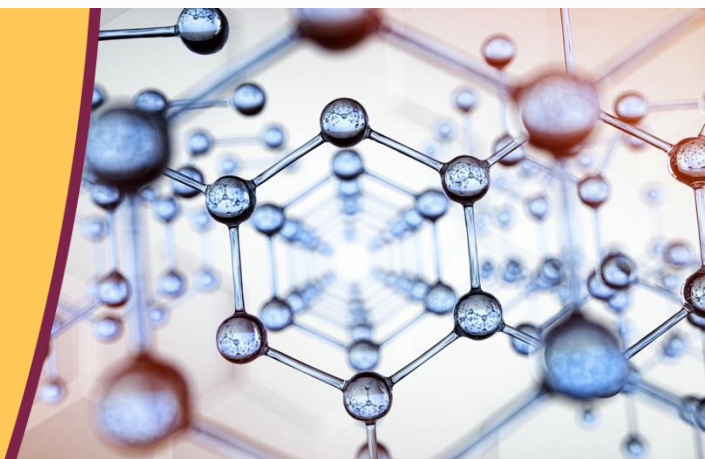- **HEC-WSI**: HPC for Wave Structure Interaction (HEC)

New Communities

- **CCP-ParaSolS** - Particulate Solids
- **CCP-AHC** - Arts, Humanities, Culture
- **CCP-DCM** - Data-driven Computational Mechanics
- **CCP-VEM** - Volume Electron Microscopy
- **UKNR** - Numerical Relativity
- **CCP-TEPP** - Theoretical and Experimental Particle Physics

CCP-QC: Quantum Computing

CoSeC & CCP-TEPP

Collaboration Aims

- CoSeC is designed as an integrated element of the community
- Over 2025 we want to form a working relationship with CCP-TEPP by:
  - Helping to identify practical technical objectives in terms of computational research
  - Creating a team of Research Technical Professionals (i.e. RSE's, computational scientists) with complimentary research aims and capabilities – starting with a CoSeC Project Lead
- Over 2026 we want to then build on this by actively participating in community activities
- CCP-TEPP can help by:
  - Engaging with CoSeC events such as its Community Forum (4th June)
  - Considering where an STFC RTP team fits into the community
  - Keeping communication channels open, both technically (CoSeC Project Lead) and in terms of impact (Programme Office)

CoSeC

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for Research Communities

Science and Technology Facilities Council

Scientific Computing