CoSeC: the Computational Science Centre for Research Communities

Update on Recent Activities

May 2021

Barbara Montanari

CoSeC Director

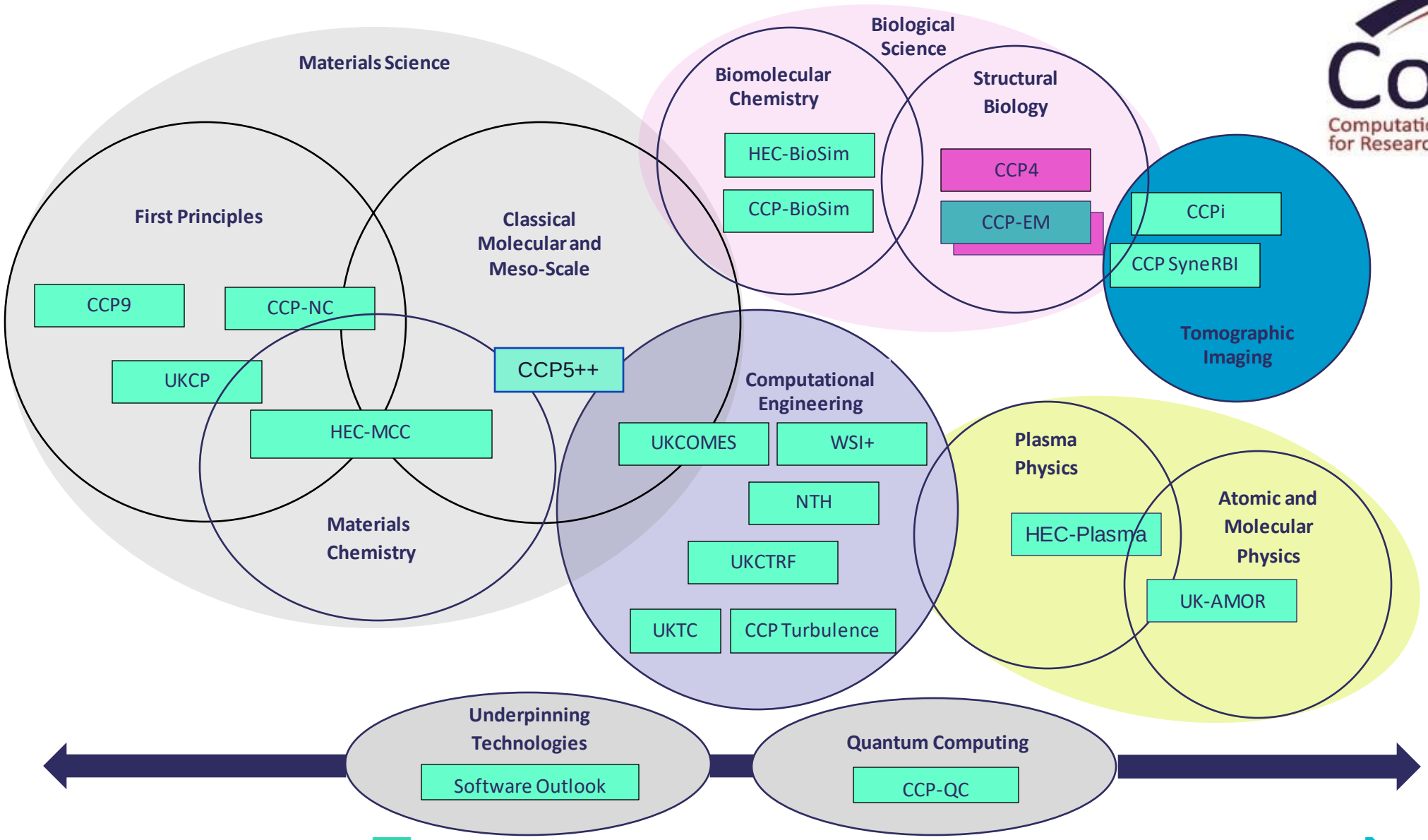
Science and Technology Facilities Council

Engineering and Physical Sciences Research Council

Biotechnology and Biological Sciences Research Council

Medical Research Council

The Landscape



CoSeC
Computational Science Centre for Research Communities

Science and Technology Facilities Council

Engineering and Physical Sciences Research Council

Biotechnology and Biological Sciences Research Council

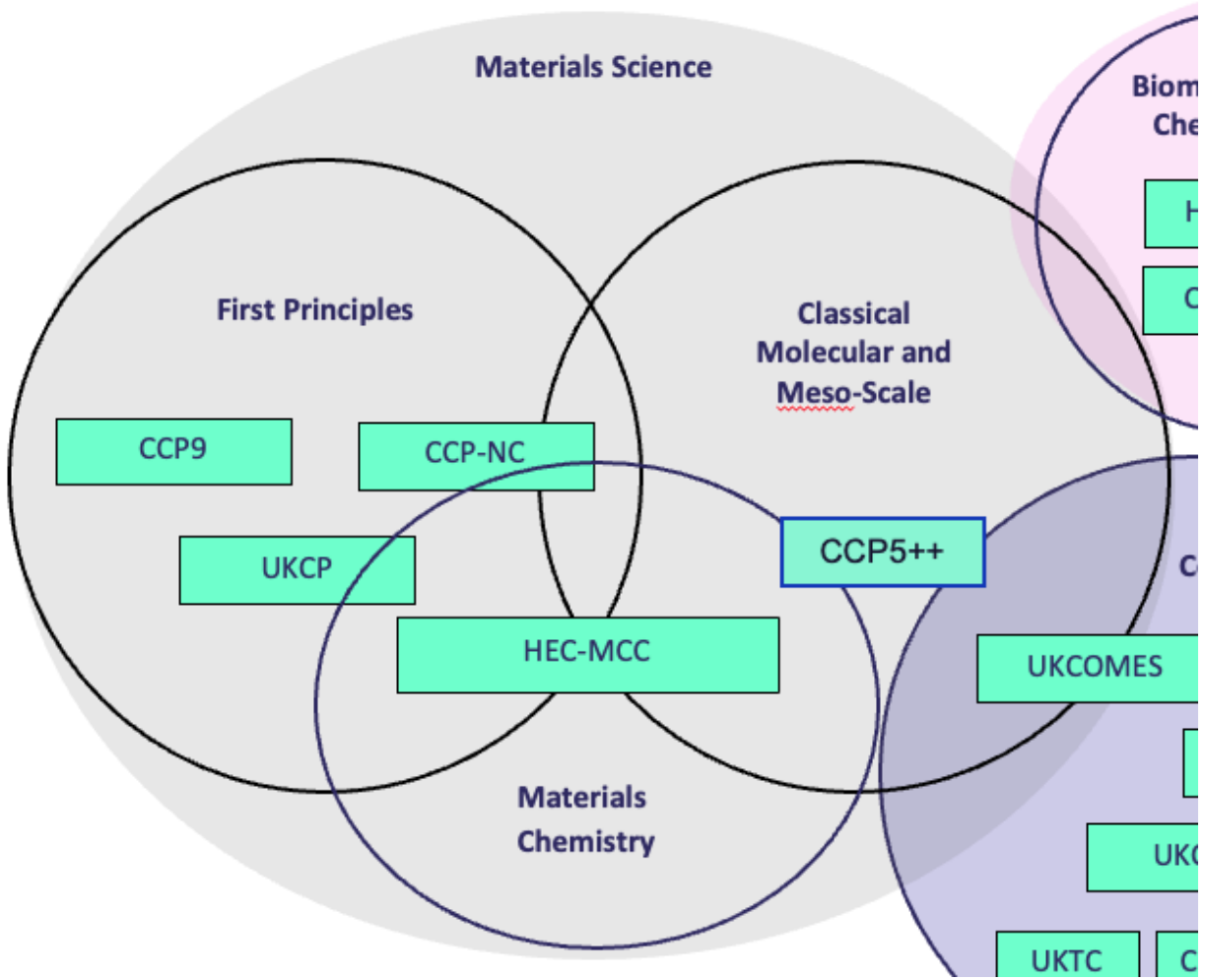
Medical Research Council

Materials Science:

- UKCP
- MCC
- CCP5++
- CCP9
- CCP-NC

Science and Technology Facilities Council

CoSeC
Computational Science Centre for Research Communities



Engineering and Physical Sciences Research Council

- **UKCP - CASTEP**:
  - Academic free-of-charge licence available worldwide.
  - CASTEP is the pilot product on STFC's new online licensing portal https://licenses.stfc.ac.uk/
  - As of 30/4/2021 183 CASTEP requests have been completed through the system, 160 of these since 11/3/2021 and the release of CASTEP 20.1.1.
  - Greatly reduced administrative burden on CoSeC staff, even at volume.
- **MCC:**
  - SAINT flagship software project completed: https://saint.chem.ucl.ac.uk/
  - Barry Searle successfully demo'd calculations on Group II oxide surfaces with probe molecules (CO, H2O and NH3)
  - You Lu/TK implemented and verified periodic QM/MM embedding with CP2K/GULP as planned.
  - New releases of DL_POLY (v5, now open source LGPL), new architecture, etc: https://gitlab.com/ccp5/dl-poly. Python companion for DL_POLY https://pypi.org/project/dlpoly-py/

Science and Technology Facilities Council

Engineering and Physical Sciences Research Council

- **ARCHER2**:
  - CRYSTAL, Tcl-ChemShell/NWChem and Py-ChemShell/NWChem are running on the 4-cabinet system

- **ExCALIBUR Working Group:**
  - *Materials and Molecular Modelling Exascale Design and Development*, April 2020 - June 2021
  - CoSeC (Ian Bush, Alin Elena and Tom Keal) continue to take part in the steering group via MCC support.
  - Focus now on developing application themes and case studies together with the community to inform phase 2 of working group.
  - IB/AE/TK are co-Is on cross-cutting grant proposal led by Matt Watkins (Lincoln) to couple atomistic and hydrodynamics methods.

CCP5 Collaborative Computational Project Computer Simulation of Condensed Phases 40th Anniversary

NEW CCP

CoSeC Computational Science Centre for Research Communities

CCP5++ Integrating Computer Simulation of Condensed Phases with experiments and data science

PI: Paola Carbone, Co-I: Alin Elena (CoSeC)

Training:

- summer school will be online, 430 applications for 120 places. New advanced lecture added on Machine Learning Potentials, lead by Gábor Csányi. Tutorials infrastructure now uses jupyter notebooks, with plan to move to cloud.
- CMake training with Edo Pasca, CoSeC support for CCPi/Synerby

Seminar series: Seminars focused on usage of molecular simulations software for modern research:

- Matteo Salvalaglio, on PLUMED
- James Kermode, on QUIP
- Richard Graham, on LAMMPS.

AGM this year merges online with MMMHUB conference with other CCPs and HECs, September, London.

UKRI Science and Technology Facilities Council

UKRI Engineering and Physical Sciences Research Council

CCP-NC

Engineering and Physical Sciences Research Council

CoSeC Computational Science Centre for Research Communities

- Published and finalised the CCP-NC database, providing a public repository for NMR computational data;
- Developed crystvis-js, a WebGL based JS 3D visualizer for solid state atomic structures, and prototyped a new interface for the next version of our flagship software, MagresView 2.0;
- Developed new tools and scripts for dipolar coupling averaging, including a new theory of 2nd moments (paper in preparation);
- Supporting an eCSE funded project, in collaboration with James Kermode from Warwick University, for the improvement and expansion of Transition State Search functionality in CASTEP

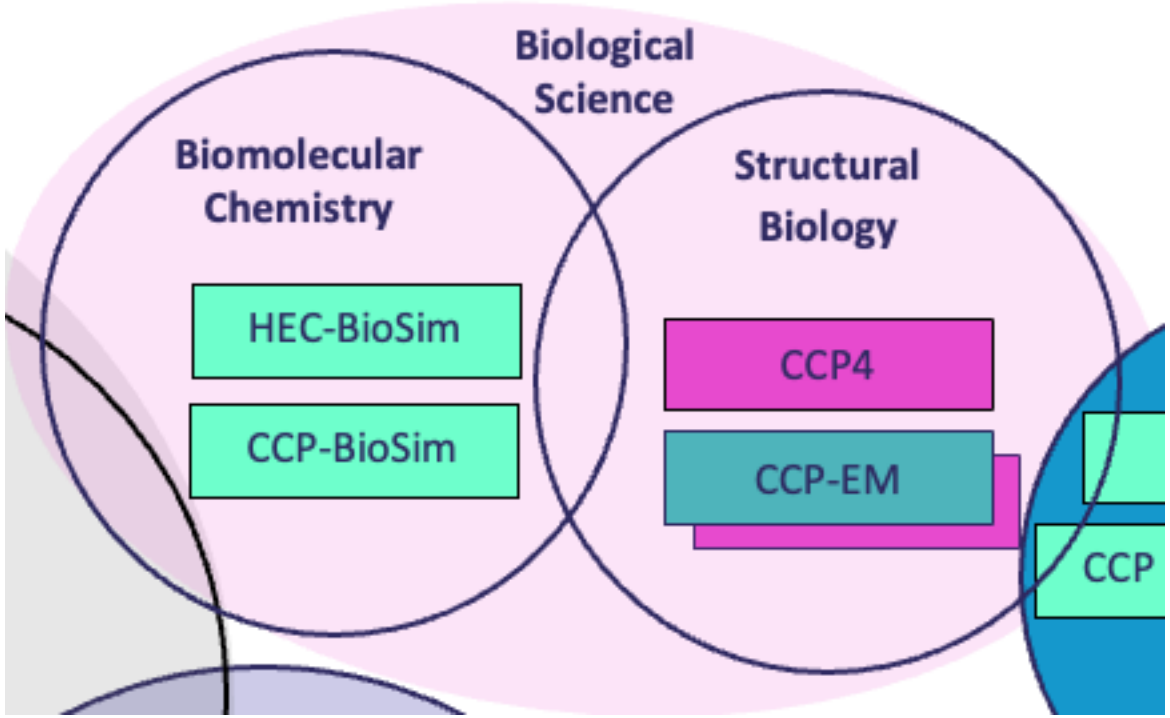
Computational Electronic Structure of Condensed Matter

Engineering and Physical Sciences Research Council

- Wannier90: build parallel and thread safe library
  - Modernization and redesign of code base
    - reworked modules, types definition and classification
  - Next steps: parallelization of library and python wrapper
- CRYSTAL support
  - Spin-orbit OpenMP parallelization completed
  - Code benchmarked on Archer2
  - CRYSTAL hands-on course tutoring
- QUESTAAL support
  - Yttrium garnet calculation with QSGW (published in EST)
  - Performed on 64 Nvidia V100 GPUs (Marconi100)
  - Awarded 46 million hours from PRACE for continuation of project
- Materials research
  - Collaboration with experiment and theory groups in India
  - Combined first-principles and magneto-transport study of YbCdSn (published in PRB)
  - Predict strongly correlated topological semimetal

Biology/Biochemistry:

- HEC Biosim
- CCP Biosim
- CCP4
- CCP-EM



Science and Technology Facilities Council

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Engineering and Physical Sciences Research Council

Biotechnology and Biological Sciences Research Council

Medical Research Council

- Support the Hartree Centre (JADE2) and N8 CIR (Bede) with opening of new Tier2:
  - Compiled biomolecular simulation codes on JADE2 and Bede
  - Supported HC with the acceptance testing of JADE2, this involved devising tests, running them and presenting the results to Oxford at the acceptance test meeting
- UK wide HPC outlook for biomolecular simulation
  - Large scale benchmarking of ARCHER2, Bede, JADE/JADE2, Dirac, ISAMBARD, THOMAS – now published on the HEC website
  - Example scripts to run on ARCHER2, JADE, JADE2 and Bede – now published on the HEC website
  - Updated benchmark suite to extract best performance from different architectures.
  - A completely redesigned suite of web pages covering access to ARCHER2, JADE, JADE2 and Bede with a single point of application and advice for PIs on how to increase chances of success – all + above now available under the “Access HPC” tab on the HEC website.
- Preparation work for the upcoming release of Longbow 2.0
- Dealing with a large volume of requests for specialist support amongst our early test groups on ARCHER2, JADE2 and Bede.
- Supporting users and PIs with the transition of their projects from ARCHER to ARCHER2.

4th CCP5/CCPBioSim Multiscale Modelling Conference, 29-31 March 2021

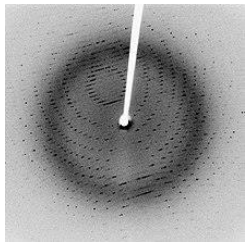
- Organised by CoSeC, D. Cole, and A. Bronowska (Newcastle)
- Held online with 400 registered participants (more than the first three events put together!).
- Included a community engagement event on STFC's ChemShell multiscale QM/MM software

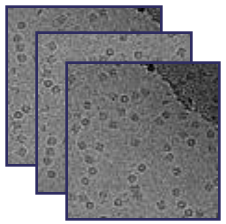
- Software development:
  - Implementation of FFEA method in Code_Saturne progressing well: new scheme under development for increased robustness than in original implementation (see CCP-EM slide)
  - Project to integrate ChemShell QM/MM functionality with "Enlighten" toolkit for protein-ligand simulations, with the aim to provide an easy-to-use graphical interface for multiscale simulation
  - Coarse-grained and atomistic MD calculations of membrane-bound P450s are complete (papers in preparation)
  - SlimMD database of MD trajectories for educational use now accessible from the CCPBioSim website

Biotechnology and Biological Sciences Research Council

CCP4 and CCP-EM

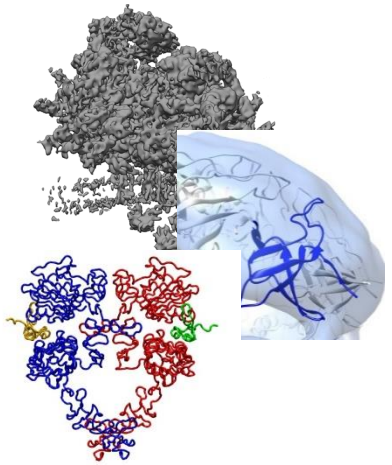
Medical Research Council





CCP4

CCP-EM



PDBe
Protein Data Bank in Europe

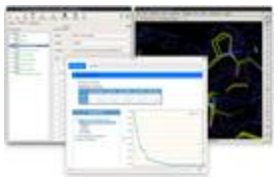
EMDataBank
Unified Data Resource for 3DEM

Methods Development

Particle picking
Diffraction data proc
Molecular replacement
Map interpretation
Metrics / validation
Machine learning

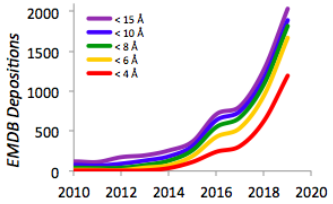
Software

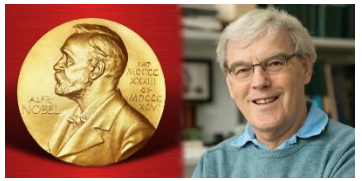
Collate software from us and collaborators.
Distribute worldwide.
Academia & pharma.



Community

CCP4 Study Weekend
CCP-EM Spring Symposium
Training
Standards



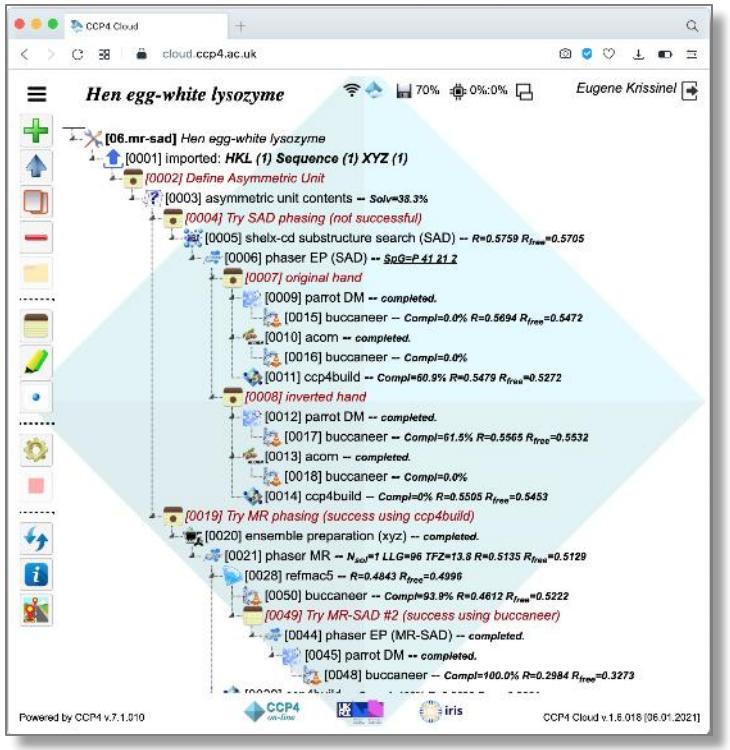


CCPBioSim

Drug design
Modelling / simulation
Function prediction
Derived databases
Ligand screening

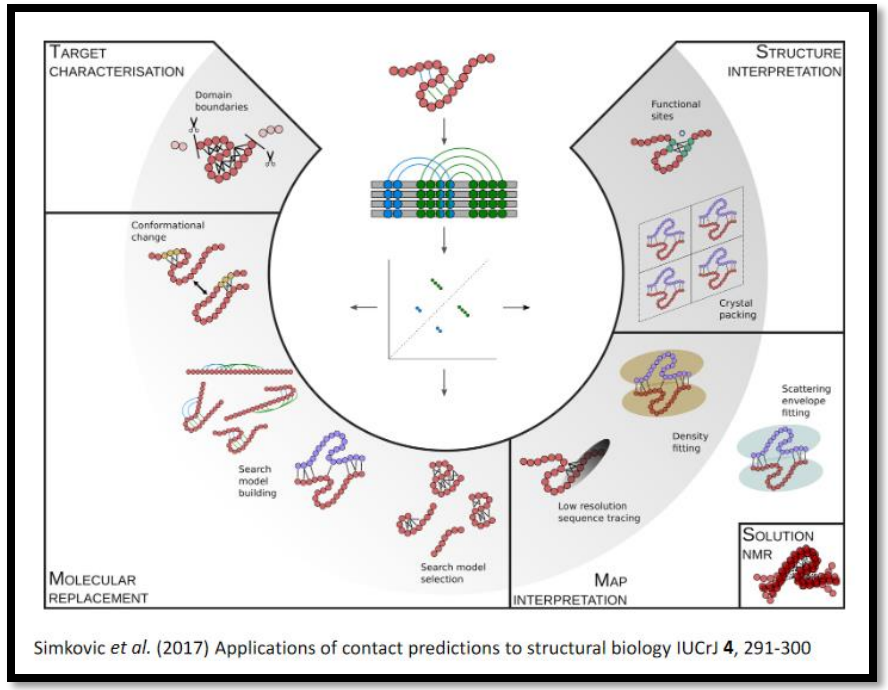
Bioinformatics in CCP4

https://cloud.ccp4.ac.uk



- Aid less experienced structural biologists
- Pushing the limits of automation
- Runs on STFC Cloud
- Used for CCP4 training courses

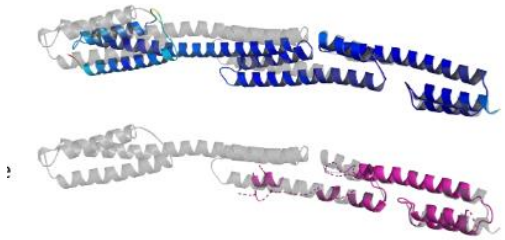
Contact predictions from large sequence alignments.
ConKit library.



Simkovic *et al.* (2017) Applications of contact predictions to structural biology IUCrJ **4**, 291-300

MRparse
Decision assistant for structure solution via Molecular Replacement.

Structure prediction.
AlphaFold2 models combined with diffraction data.
GREMLIN, PConsFam databases.



T1030. 3.03 Å
Solves with 18-44% truncated versions

UNIVERSITY OF LIVERPOOL

CCP-EM

CoSeC
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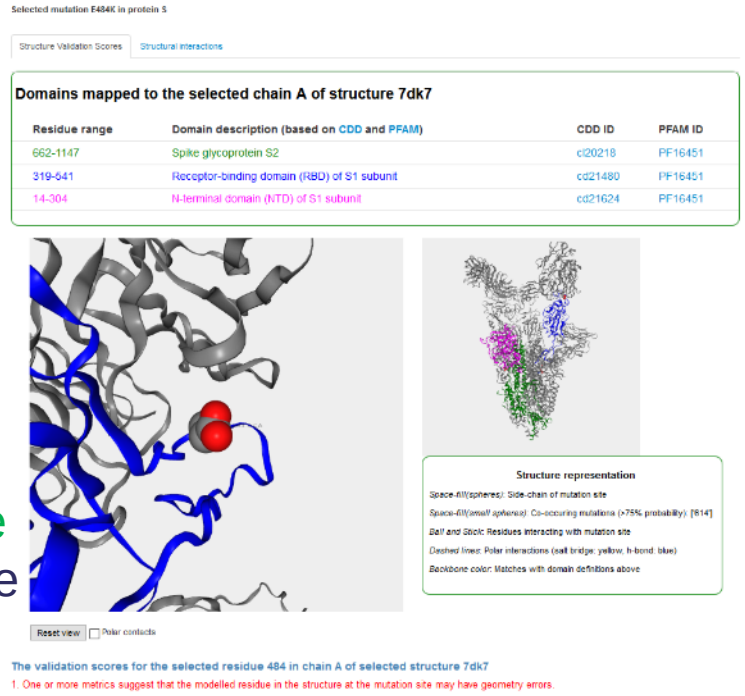
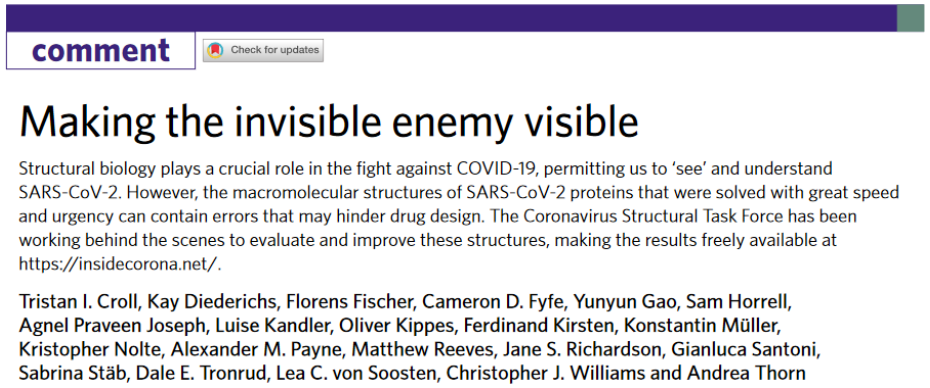
SARS-CoV-2

CoVal server
coval.ccpem.ac.uk
Links variants to structure
Working with COG-UK

Coronavirus Structural Task Force
Use of CCP-EM validation pipeline
Nat Struct & Mol Biol.




comment
Check for updates

Making the invisible enemy visible

Structural biology plays a crucial role in the fight against COVID-19, permitting us to 'see' and understand SARS-CoV-2. However, the macromolecular structures of SARS-CoV-2 proteins that were solved with great speed and urgency can contain errors that may hinder drug design. The Coronavirus Structural Task Force has been working behind the scenes to evaluate and improve these structures, making the results freely available at https://insidecorona.net/.

Tristan I. Croll, Kay Diederichs, Florens Fischer, Cameron D. Fyfe, Yunyun Gao, Sam Horrell, Agnel Praveen Joseph, Luise Kandler, Oliver Kippes, Ferdinand Kirsten, Konstantin Müller, Kristopher Nolte, Alexander M. Payne, Matthew Reeves, Jane S. Richardson, Gianluca Santoni, Sabrina Stäb, Dale E. Tronrud, Lea C. von Soosten, Christopher J. Williams and Andrea Thorn

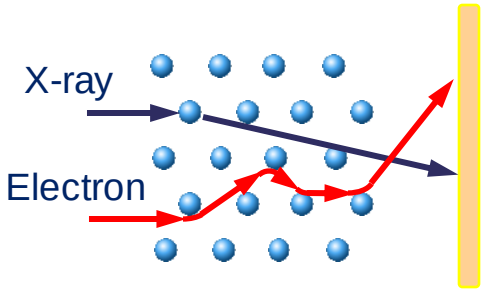
CCP-EM Symposium

Attendance: 290 (2019), ~3000 (2020), ~2000 (2021)
Talks on YouTube.
Proceedings in Acta Cryst. D

Future directions

Electron diffraction

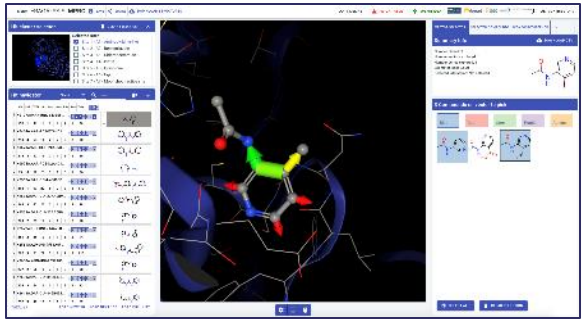
Interest for nano-crystals
Multiple scattering
WP in CCP4 grant
Simulations of e^- - crystal interactions.



Fragalysis

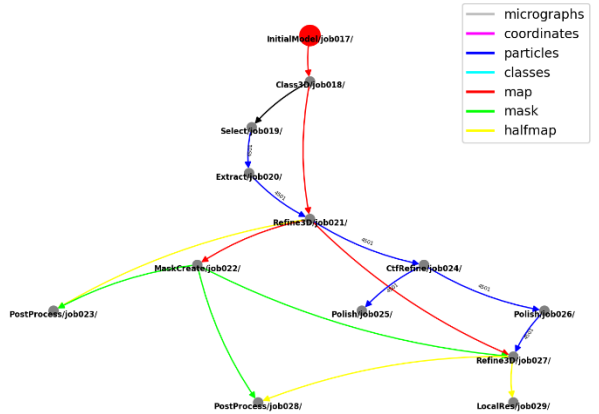
fragalysis.diamond.ac.uk

Analyzing large amounts of protein-ligand data from fragment screening (XChem).
Link to medicinal chemistry.



New grant

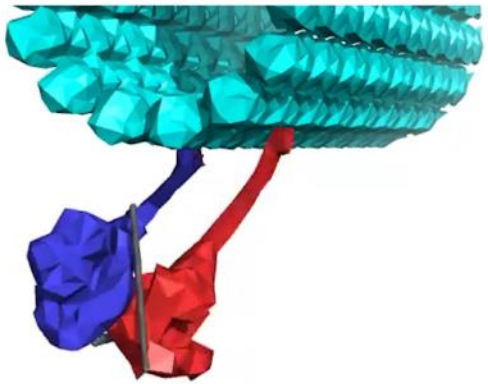
Themes: machine learning, tomography
Pipeliner project.
Metadata tracking and data annotation for validation / deposition / M-L training.
Volume EM
Links to cell / tissue community
www.volumeem.org



Pipeliner – workflow analysis

FFEA

Meso-scale modelling of cryoEM volumes
Sarah Harris @ CCP4 SW 2020
CCP-BioSim, CCP-EM, CCP4, Comp Eng @ DL



Science and Technology Facilities Council

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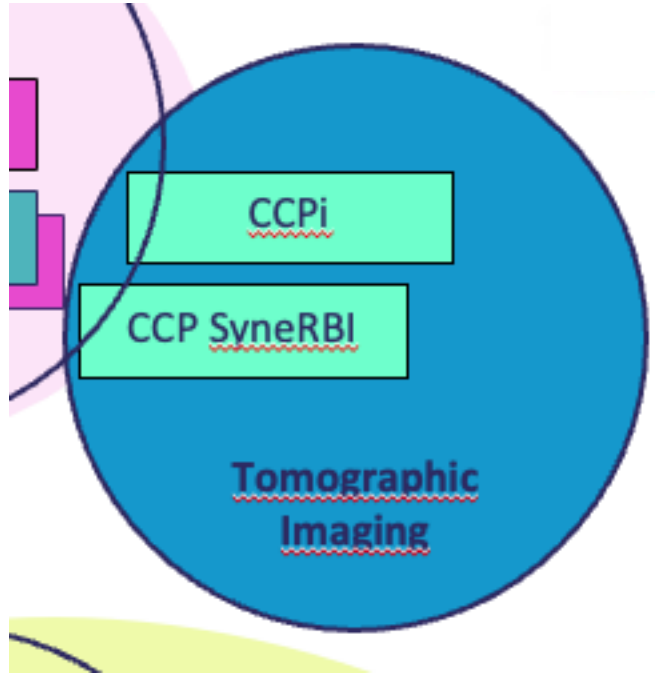
Computational Science Centre for Research Communities

Tomographic Imaging

- CCPi
- CCP SyneRBI



Engineering and Physical Sciences Research Council

CCP Tomographic Imaging – CCPi

CCP SyneRBI – Synergistic Reconstruction for Biomedical Imaging

Open Source Software

- **S**ynergistic **I**mage **R**econstruction **F**ramework (SIRF), platform for implementation and validation of novel reconstruction algorithms in multimodal imaging (PET/MR)
- **C**ore **I**maging **L**ibrary (CIL): a versatile framework for tomographic imaging
- CCPi **Regularisation**: routines for iterative image reconstruction
- **D**igital **V**olume **C**orrelation: technique for analysis of 4D tomographic imaging
- **CILViewer**: 3D interactive viewer

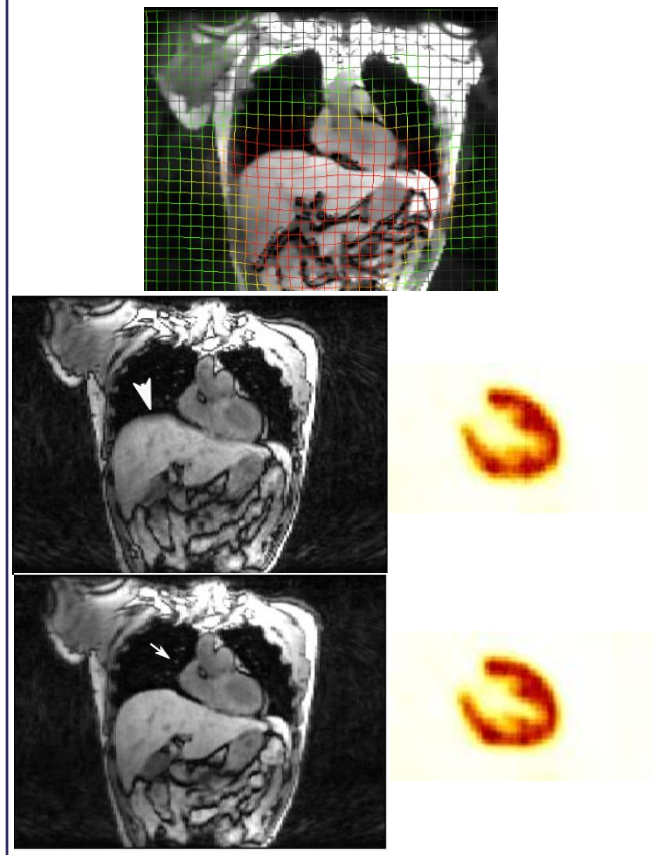
Outreach

Training school on SIRF and CIL:
- 2019: 50 participants (2 days @ Daresbury)
- 2021: 120 participants (online) part of Fully3D conference

Scientific output:
- 2020: 2 peer review articles
- 2021: 5 peer review articles
- Contributions to workshops and conferences

Networking

- Synergistic Reconstruction Symposium November 2019 (Chester)
  100 participants (2 days scientific program) co-organised with CCP SyneRBI
- PET/MR User's Meeting 2020: technical challenges (London)
- Workshop: **D**igital **V**olume **C**orrelation analysis: state of the art and applications in material science (online)
  2pm-6pm 26 May 2021



Example reconstructions for cardiac Magnetic Resonance and Positron Emission Tomography where respiratory motion is determined from MR data (top). Reconstructions without motion correction (middle) are compared to motion-compensated reconstructions (bottom). Data reconstructed with software from CCP SyneRBI and CCPi in a collaboration between 3 different UK universities, CoSeC and institutions in Germany and Australia.

UKRI Engineering and Physical Sciences Research Council

CoSeC Computational Science Centre for Research Communities

- Computational Engineering
- UKTC
- UKCTRF
- UKCOMES
- CCP WSI+
- CCP NTH
- CCP Turbulence

Science and Technology Facilities Council

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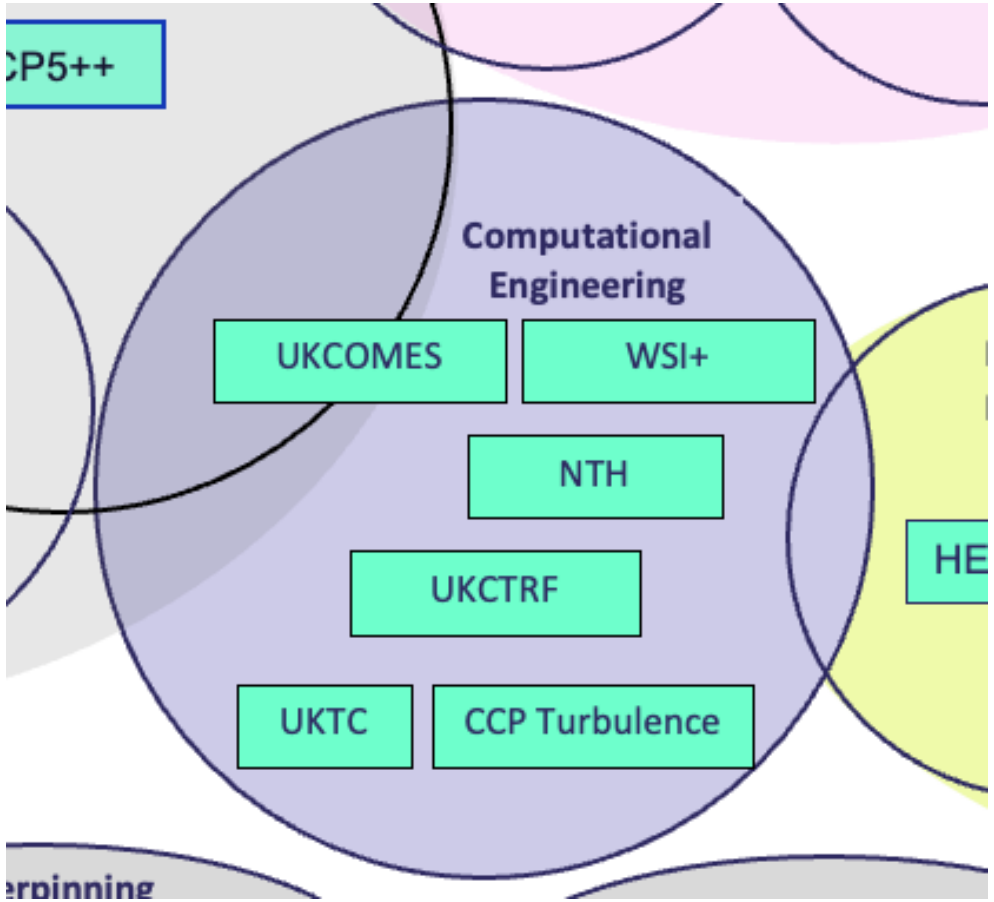

Engineering and Physical Sciences Research Council

Collaborative Computational Project in Nuclear Thermal Hydraulics (CCP-NTH)

NEW CCP

CoSeC
Computational Science Centre for Research Communities

Code Development:

- Released the community thermal hydraulic DNS code (CHAPSim1.0), which carries out DNS modeling of supercritical water/CO2 or liquid metals with unique heat transfer characteristics
  - CHAPSim1.0 tested in the 4-cabinet system of ARCHER2
- Development of CHAPSim2.0, code-refactoring
  - Added high order spatial discretization (from the 2nd order of CHAPSim1.0 to the 6th order c CHAPSim2.0) to capture subtle characteristics with limited numerical dissipation for a bette fundamental study of turbulence and heat transfer/
  - (on-going) Reconstruction of the code parallelization from 1-D to multi-dimensional parallelization to make complete usage of the latest advanced HPC systems (i.e. ARCHER

Training & Seminars:

- A training course on Nuclear thermal hydraulics modelling using *Code_Saturne*, jointly organise by PRACE, CCP-NTH, CCP Turbulence on 10-11 March 2021.
- Regular CHAPSim Users Meetings
- Regular CCP-NTH special topic seminars.

A website on STFC server was created for CCP-NTH. (www.ccpnth.ac.uk)

UKRI Engineering and Physical Sciences Research Council

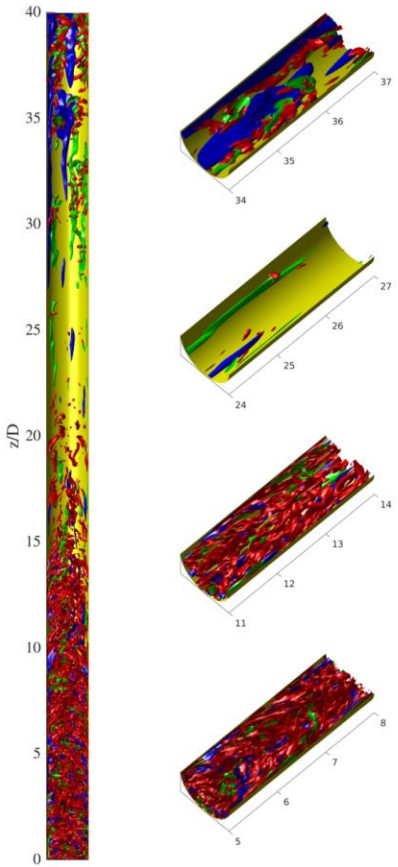

Fig: CHAPSim1.0 simulation of supercritical CO2 laminarization and turbulence regeneration in an upward pipe flow under effect of buoyancy and variable properties.

CCP-WSI
a Collaborative Computational Project in Wave Structure Interaction

NEW CCP

CoSeC
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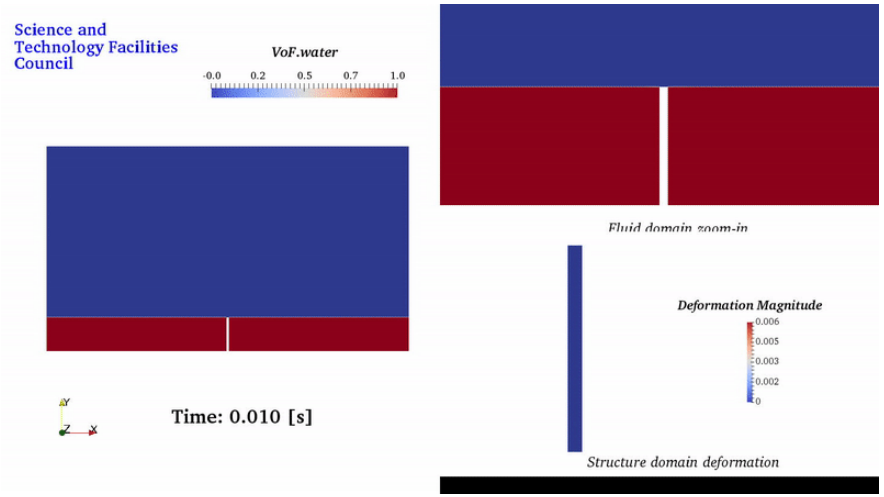
- Code Developers Workshop held virtually 7th-8th April 2021 (https://tinyurl.com/2nhjymjh):
  - 15 speakers over 2 days
  - Wide variety of WSI-related software development topics
- Significant website update for renewed CCP (www.ccp-wsi.ac.uk):
  - All content brought up-to-date
  - Code and data repositories tidied up
  - New initiative underway to create a CCP-WSI software catalogue
- New general-purpose partitioned FSI framework released:
  - https://github.com/parMupSiF/parMupSiF
  - Building on existing CCP-WSI community tools
  - The basis of a new multi-physics WSI solution



UKRI Engineering and Physical Sciences Research Council

UK TURBULENCE CONSORTIUM

UK CTRF UK CONSORTIUM ON TURBULENT REACTING FLOWS

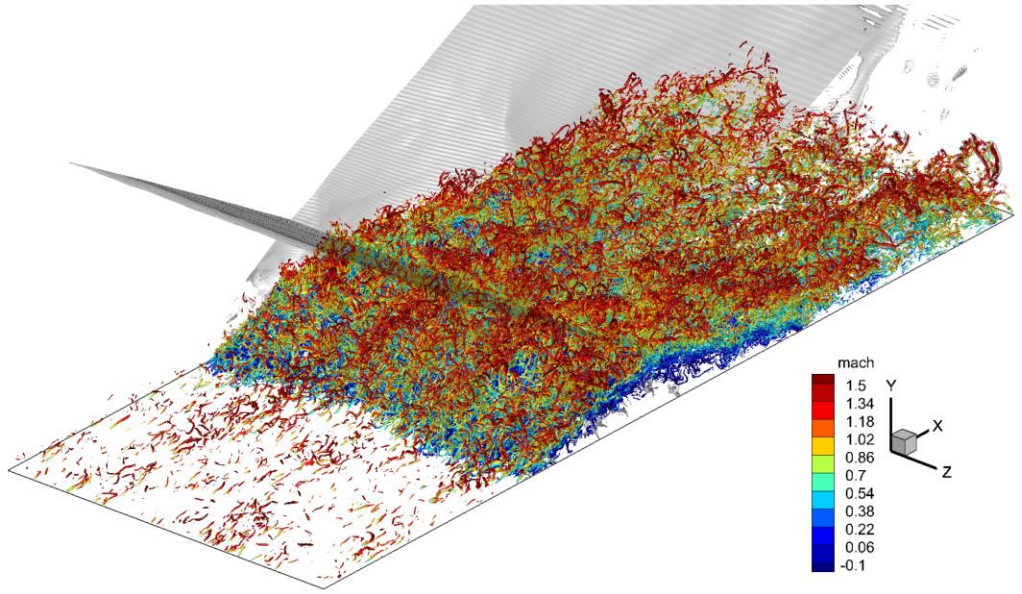
UK CONSORTIUM ON MESOSCALE ENGINEERING SCIENCES

CCP Turbulence

NEW CCP

CoSeC Computational Science Centre for Research Communities

- **UKCOMES**:
  - Organised ExCALIBUR workshop (Luo and Meng).
  - Collaborating with Cambridge and UCL on developing the use case of coupling lattice Boltzmann method and finite element method.
  - Signficant performance improvements made to MPLB when running on GPU-based systems, enabling larger scale LBE simulations on modest computing resources (~100X over a single CPU core)
  - New LBE algorithm developed for 3D non-spherical drops as fluid-filled vesicles (with applications including e.g. red blood cells): article ready for submission and implementation for DL_MESO in progress
- **UKCTRF**:
  - SENGA introduction of HDF5
  - Parallel Adaptive Mesh Refinement (PAMR) software library
  - Benchmarking and on-going validation of HAMISH.
  - Annual workshop held online
- **UKTC/CCP Turbulence**:
  - Code_Saturne training course held March 2021
  - Jian Fang won the UKTC video competition (see image)
  - Optimisation of the sequential part of Xcompact3d



UKRI Engineering and Physical Sciences Research Council

Miró, A., Soria, M., Cajas, J. C., Rodríguez, I., & Moulinec, C. (2021). Flow topology and heat transfer analysis of slotted and axisymmetric synthetic impinging jets. International Journal of Thermal Sciences, 164, 106847.

UK TURBULENCE CONSORTIUM

UK CTRF UK CONSORTIUM ON TURBULENT REACTING FLOWS

UK CONSORTIUM ON MESOSCALE ENGINEERING SCIENCES

CCP Turbulence

NEW CCP

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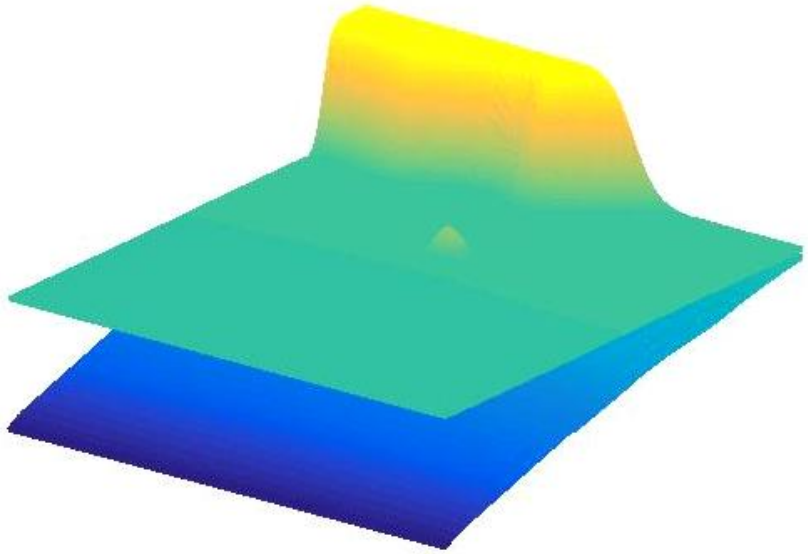
- **ExCALIBUR Working Groups:**
  - **UKCOMES**: Exascale Computing for System-Level Engineering: Design, Optimisation and Resilience.
  - David Emerson, Jianping Meng and Luke Mason from STFC Daresbury Co-I's.
  - **UKTC/CCP Turbulence**: Turbulent Flow Simulations at the Exascale: Application to Wind Energy and Green Aviation (David Emerson Co-I)
- **eCSE projects:**
  - **UKTC/CCP WSI+/CCP Turbulence**: A Partitioned Fluid-Structure Interaction Framework for Exascale. Project will couple Code_Saturne and FEniCS to tackle large-scale FSI problems (9 months of STFC effort, Wendi Liu, Alex Skillen, Charles Moulinec from STFC Daresbury Co-I's)
  - **UKCOMES**: Multi-Resolution Coupling for Exascale Engineering (6 months of STFC effort, Alistair Revell (PI, University of Manchester) with Charles Moulinec, Jianping Meng and Chrysovalantis Tsinginos)
- **ARCHER2**:
  - **UKTC/UKCTRF/CCP Turbulence**: Early access identified a problem with the interconnect and MPI AlltoAll command.
  - **CCP-NTH**: Pioneer project approved: High-Fidelity Simulations to Improve Performance and Safety of PWRs with Charles Moulinec and Wei Wang

UKRI Engineering and Physical Sciences Research Council

- **Training events**:
  - Horizon 2020 E-CAM Extended Software Development Workshop in HPC for mesoscale simulation (held online): seminar and practical exercises on mesoscale modelling and DL_MESO delivered by Michael Seaton, January 2021
  - Usage of HiLeMMS interface and its backend to MPLB (held online): one-on-one training to members of Institute for Materials and Processes, Edinburgh University delivered by Jianping Meng, March 2021
  - Horizon 2020 E-CAM/CECAM Industry Training at the Mesoscale: seminar and practical exercises on DPD and DL_MESO delivered by Michael Seaton, April 2021



Simulation for a laboratory scale model ($205 \times 6 \times 3.4$ m - 1:400) of the tsunami runup near the village of Monai in Okushiri Island, Japan, conducted using MPLB

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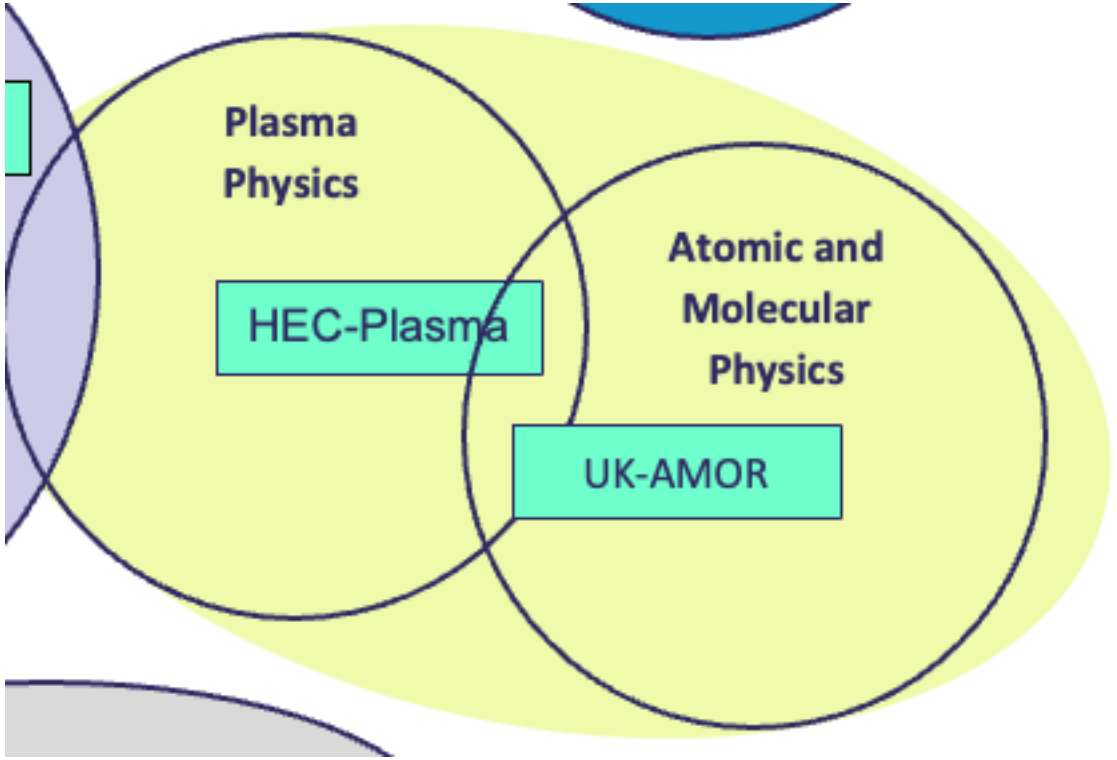
Atomic, Molecular, Optical, and Plasma Physics:

- UK-AMOR
- HEC-Plasma



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HEC-Plasma UK AMOR

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Joined UK-AMOR and HEC-PLASMA workshop (with CCPQ and CCP-PLASMA):

Atomic and Molecular Data Needs for Plasma Applications

13-15 April 2021, online (postponed from a planned meeting last year due to COVID)

- 160 registered international participants, 23 speakers from AMO physics (and chemistry) and diverse plasma applications, discussion sessions (fusion, low-temperature plasmas, accurate and comprehensive collision data sets and their uncertainties), a demonstration of industrial code tools (Quantemol Ltd) and poster sessions.
- A workshop bringing together the two scientific communities, with scientific, industrial and energy research applications in nuclear fusion, nanolithography, chemical engineering and astrophysics which require varied and accurate atomic and molecular physics data.
- The talks and posters will be preserved on the CCPQ website, and a citable summary proceedings document will be put together on STFC's 'epubs' site.

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HEC-Plasma UK AMOR

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- CoSeC work continued supporting the new projects (eCSE, laser-atom double-ionization EPSRC grant AquA-DIP) discussed at the previous meeting and as well as plans for a new low-energy antimatter (antihydrogen interactions) proposal related to ongoing (necessarily slow but steady) coding for the ultralow temperature reactive molecular collision code package RMAT_REACT.

- ARCHER2 benchmarking by CoSeC of PLASMA codes GS2 and Bout+, and porting and testing of QUB antimatter (many-body theory) positron-molecule code package ANTI-ATOM (in advance of a new grant application).

- Congratulations to QUB's Dr Andrew Brown on gaining an EPSRC Research Software Engineering Fellowship. CoSeC's M Plummer is a project partner. This project will build on, follow up and greatly expand on code curation, integration and development work of electron collision and multiphoton ionization codes at QUB (in particular) and more generally as performed until now through the lifetime of CCPQ and UK-AMOR.

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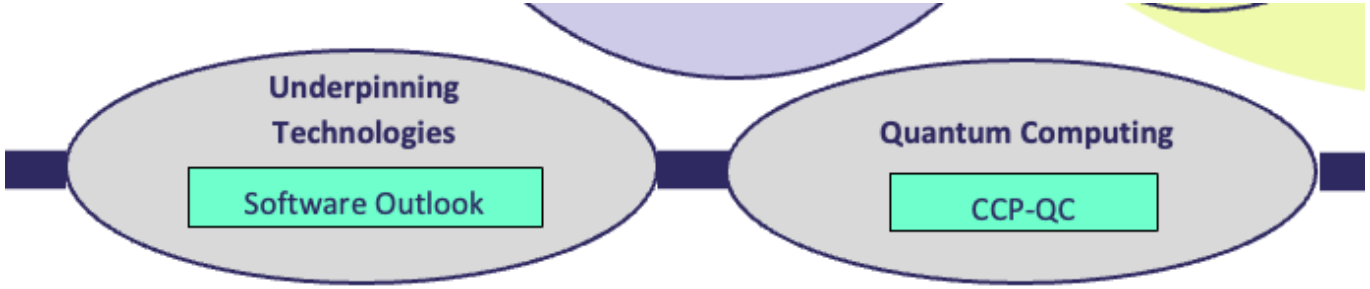
Cross-cutting/underpinning:

- CCP QC
- Software Outlook



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CCP-QC

NEW CCP

in Quantum Computing

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- **WG2**: Crystallography meets quantum computing, working group meets regularly driven by the problem provided by Ronan Keegan (CCP4) and solution coming from QC Adam Callison (UCL) and Nicholas Chancellor (Durham) between others.

Outreach talks, hosted at a virtual DL:

- Quantum control stacks - why do need more control? by Marco Ghibaudi, Riverlane, March 9, 2021 (online), https://youtu.be/vBNAVdo5OJ0/
- Estimating Partition Functions: A Quantum-Inspired Classical Algorithm, Dr Animesh Datta, University of Warwick, 18 of May 2021, https://youtu.be/MnJxMC_m91k

Workshops:

- Integrating Quantum Computers in Condensed Matter Physics Simulations National Physical Laboratory, 23th-24th September 2021, https://ccp-qc.ac.uk/qc_cm/
- another workshop on same topic was accepted at EPS-CMD/IOP Biannual conference, August 2022, Manchester.

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Software Outlook www.softwareoutlook.ac.uk

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Best Practice Guides

- Version Control Systems
- Continuous Integration, Deployment and Delivery
- Code Containers
- Documentation Tools and Best Practices
- Code Testing (In preparation)

FAIR Software Metrics: International Working Group

Mathematical libraries: linear algebra

- Simulations often limited by solution of linear algebraic systems
  - time and memory limitations
- Compare different preconditioning libraries (i.e. transformation into equivalent but faster to solve problem)

ExCALIBUR NEPTUNE Preconditioning Project

Code Coupling

- Simulations becoming more complex: couple codes together
- Multiple coupling libraries available. Compare
  - HPC scalability
  - Ease of use
  - Suitability for different types of coupling
- Report (in preparation)
- CoSeC Working Group on Code Coupling
  - Presentation given in May

GPGPU Frameworks

- Comparison of frameworks for utilising GPGPU
  - CUDA, OpenACC, OpenCL, OpenMP (Kokkos and SYCL comparison in another project: in preparation)
- Technical Report
  - Comprehensive resource for members of the scientific computing community
  - Guide in identifying the best approach to deploy when porting scientific codes
    - Productivity and performance

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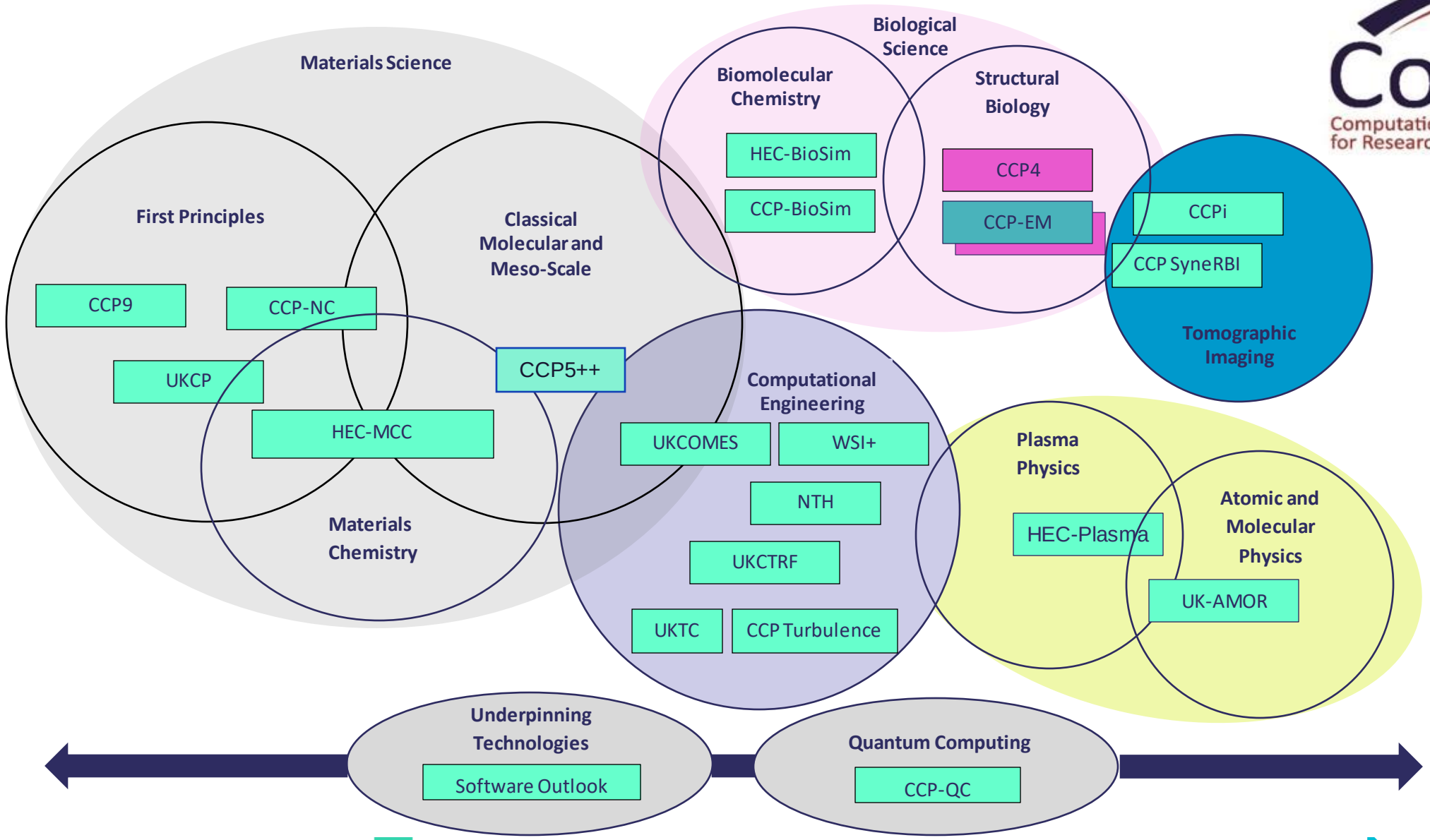
The Landscape



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Medical Research Council

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Impact Activities

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Impact

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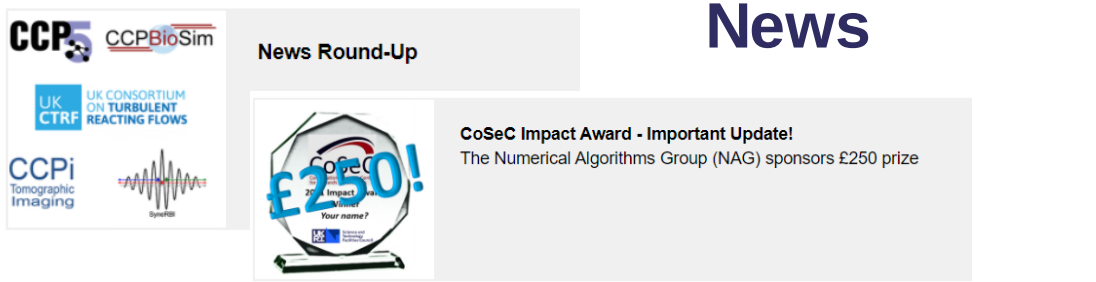
Impact Award

	2021	2020
# Applicants	12	9
# Top-ranked applications	4 (1st, 2nd, 2 x 3rd)	3 (1st, 2nd, 3rd)
Monetary prize?	£500 (Thanks to NAG - £250, £100, 2 x £75)	No

- News article announcing results (shared with NAG) and tweet*
- 4 Case Studies
- Award 'presentation' later this year

News



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215 followers ← increased from 184 in Nov 2020

Website / Pages

CCP/HEC migration from Drupal 7 to new platforms

1. Website owners explore the demo platforms and confirm choice by 30th June, 2021
2. All website owners will have chosen platform available in their own sandbox for thorough testing before going live
3. Old sites decommissioned/archived (1st March 2022)

CoSeC Web pages

We can now use : http://www.cosec.stfc.ac.uk/

Re-design underway

Consult project leaders re content

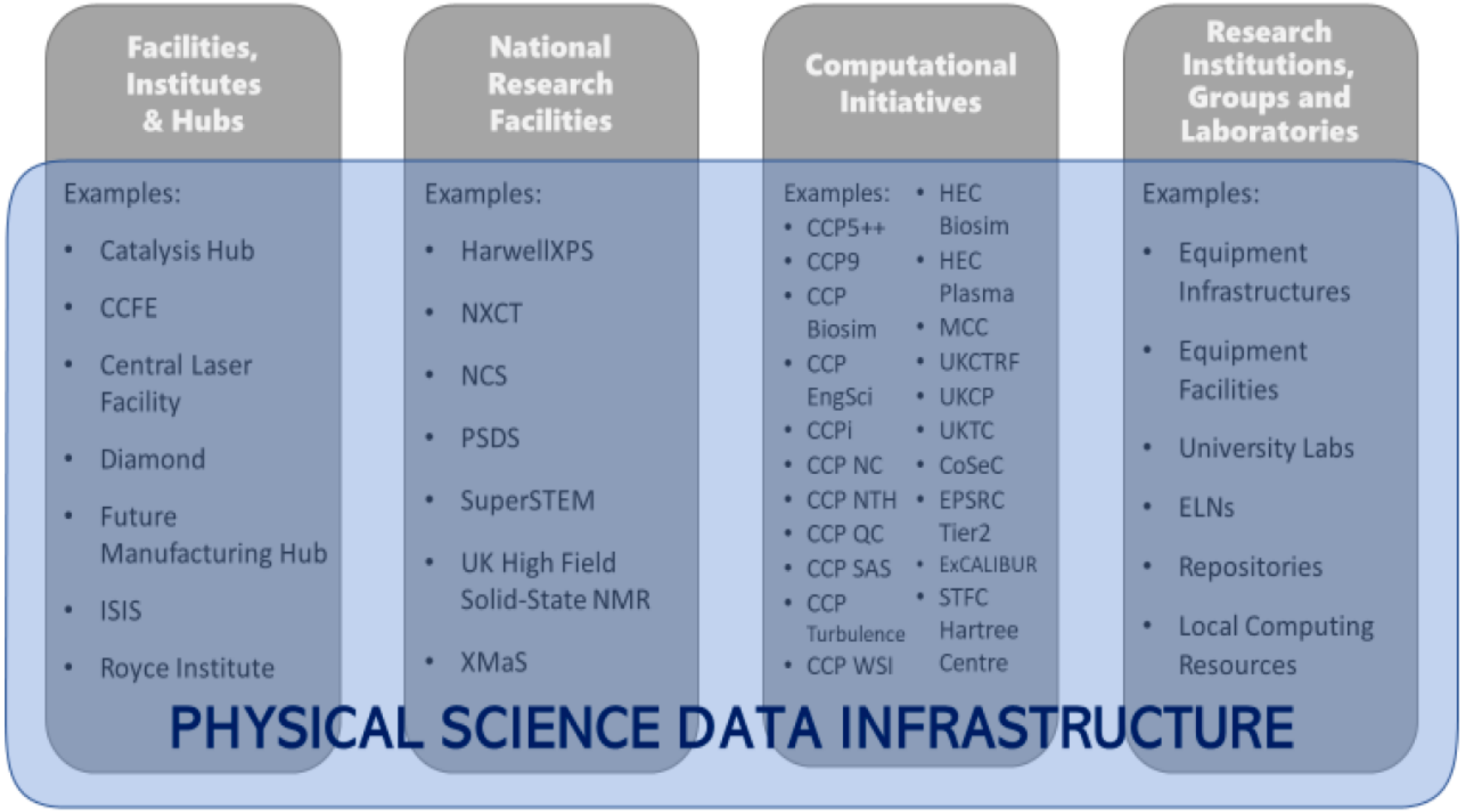
CoSeC
Computational Science Centre for Research Communities

Just one more thing …

Photo: NBC

PSDI

- Access to reference quality data
- Data, software and model sharing
- Combining data from different sources
- Close-to-data computation and containerization of data and software
- Artificial intelligence in research and innovation
- Open Research



Statement of Need submitted to EPSRC Large Scale Infrastructure, submitted Feb ’21 on behalf of of most of you et al.
S. Coles, J. Frey, N. Knight (Southampton), B. Montanari, J. Bicarregui, B. Matthews, V. Bunakov (STFC)

Conclusions

- CoSeC has a wealth of expertise and established collaborative relationships with many research communities across a broad range of subjects in the UKRI landscape
- CoSeC supports tens of thousands of researchers through a broad range of activities (e.g., collaborative research and software engineering, software licensing, distribution and support, training, community coordination and more!)
- CCPs and CoSeC are proven effective mechanisms to develop and support research across UKRI

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A big applause to the CoSeC people:

Leon Petit, Barry Searle, Martin Plummer, Gilberto Teobaldi, Jerome Jackson, Simone Sturniolo, Edoardo Pasca, Evangelos Papoutsellis, Gemma Fardell, Evgueni Ovtchinnikov, Alin Elena, Tom Keal, James Gebbie, Kakali Sen, Ya-Wen Hsiao, Charles Moulinec, Sarah Fegan, Stephen Longshaw, Gemma Poulter, Xiaohu Guo, Stefano Rolfo, Jianping Meng, Wei Wang, Dave Emerson, You Lu, Ian Bush, Ilian Todorov, Chin Yong, Dominik Jochym, Michael Seaton, Jian Fang, Alex Skillen, Xiaojun Gu, Sue Thorne, Philippa Rubin, Sergi Siso, Vendel Szeremi, Jack Taylor, Eugene Krissinel, Charles Ballard, Ronan Keegan, David Waterman, David McDonagh, Andrey Lebedev, Oleg Kovalevsyi, Ville Uski, Kyle Stevenson, Karen McIntyre, Helen Walker, Martyn Winn, Tom Burnley, Colin Palmer, Agnel Joseph, Jola Mirecka, Alister Burt, Damian Jones, Dawn Geatches.

…and many thanks for sustained support to:

UKRI Engineering and Physical Sciences Research Council

UKRI Biotechnology and Biological Sciences Research Council

UKRI Medical Research Council