Collaborative Computational Project – Quantum Computing

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CCP-QC website: https://ccp-qc.ac.uk

CCP-QC

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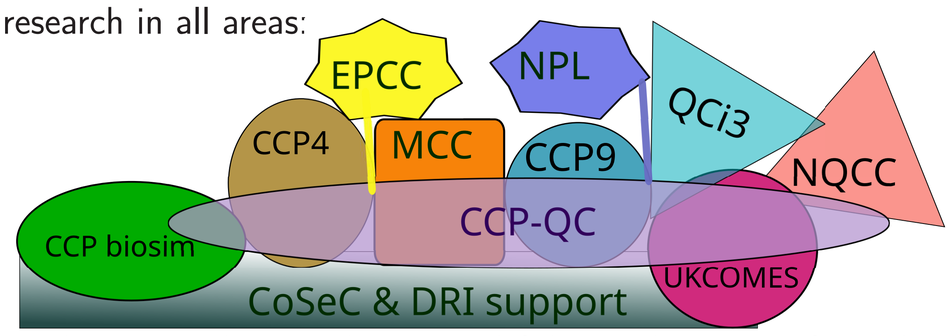
→ *ask to be added to the mailing list!*

- CCP-QC is a UKRI EPSRC-funded network linking computational scientists and engineers with quantum computing experts, to jointly develop some of the first useful applications of quantum computers.
- computational tasks in materials, chemistry, physics, biology, and engineering are developed by communities in CCPs – CCP-QC networks across CCPs and the quantum computing community.
- CCP-QC network activities:
  - organise joint meetings with other CCPs and the quantum computing community
  - support networking events and activities, including workshops and online seminars
  - run small projects to develop proof-of-principle code and demonstrations on early quantum computing hardware, with STFC CoSeC* support
  - provide an online information resource on scientific applications of quantum computing.

UKRI Digital Research Infrastructure

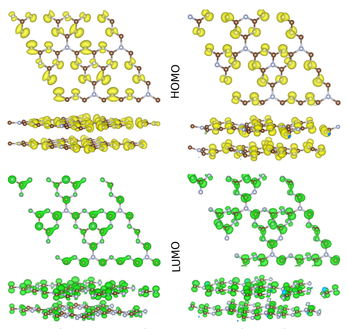
CCP funding and remit is expanding across all UKRI councils to support computational research in all areas:



CCP-QC provides a cross-cutting theme: quantum enhanced computational research across academia

∗ HEC = High End Computing Consortia ∗ CoSeC = The Computational Science Centre for Research Communities @ STFC

CCP-QC project – electronic structure calculations:



graphitic carbon nitride, showing the charge densities of the highest occupied and lowest unoccupied states, (calculated with DFT by Maruf Mridha & John Buckeridge, LSBU)

Collaboration with UKCP HEC*; CCP9 – faster and more accurate electronic structure calculations would facilitate a wide range of computational materials research, and also support biomolecular simulation (CCP biosim). *CCP Bridge project funding* to develop quantum algorithms beyond variational methods.

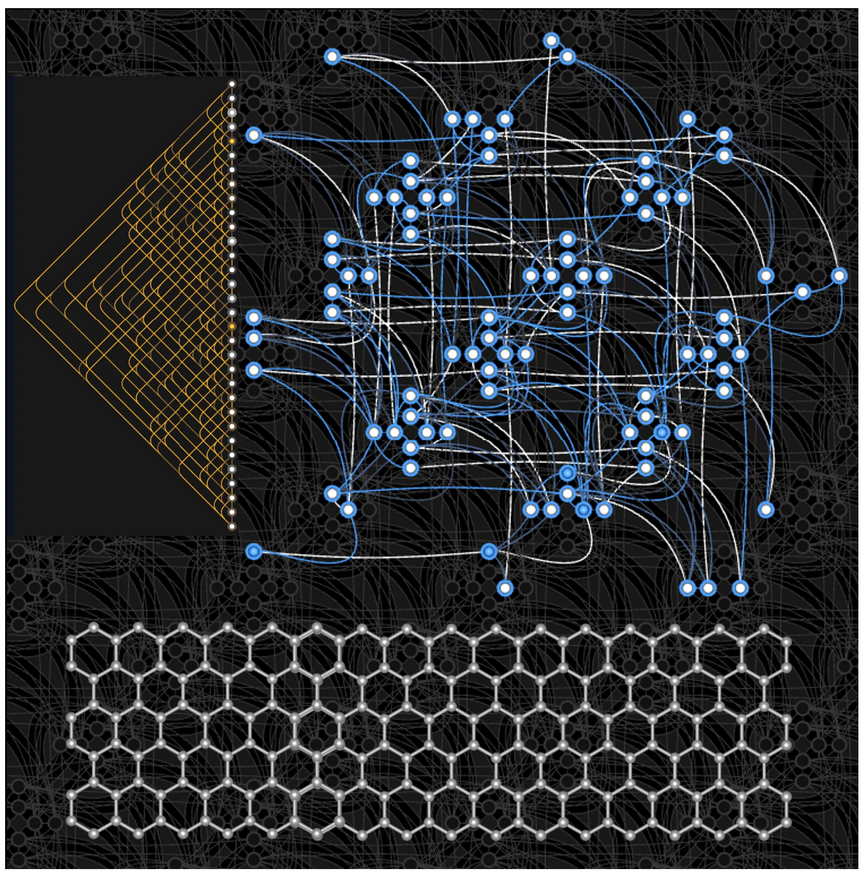
• focus on Green's functions, and implementation on neutral atom quantum computing platforms.

→ *quantum systems can naturally represent the fermionic wave functions of electrons, that are hard to optimise classically due to the sign problem*

(sign problem = fermion wavefunctions change sign under exchange of identical particles)

Royal Society Hooke Discussion Meeting:

Quantum Computing in Materials and Molecular Sciences • 6–7 Oct 2025, London



• website: *proceedings coming soon*
https://royalsociety.org/science-events-and-lectures/2025/10/quantum-computing/

graphics from D-Wave simulations of vacancies in graphene by Bruno Camino (UCL)

Review article: open access

Quantum algorithms for scientific computing
R. Au-Yeung, B. Camino, O. Rathore and V. Kendon
Reports on Progress in Physics, 2024, 87 116001
DOI 10.1088/1361-6633/ad85f0

CCP-QC is run by:

CCP-QC

Viv Kendon (Strathclyde, QCi3) – chair
Paulo Emilio Trevisanutto (STFC) – secretary
John Buckeridge (London South Bank) – deputy chair
Petros Wallden (Edinburgh, QCi3) – deputy chair

CCP Bridge project Researcher Co-Is:
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Johannes Kombe (Strathclyde)
Steph Foulds (Strathclyde)

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Stewart Clark (Durham, CCP9 chair)
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Gabriele De Chiara (QUB, CCPQ)
Alin Marin Elena (STFC)
Sarah Harris (Sheffield, CCP biosim chair, QCi3)
Peter Haynes (Imperial, CCP9, UKCP, QCi3)
Dieter Jaksch (Hannover)
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Steven Lind (Cardiff, QCi3)
Ivan Rungger (NPL, QCi3)
James Thorne (NQCC)
Scott Woodley (UCL, MCC chair)

Advisory Team:
Sir Richard Catlow (Cardiff, UCL, MCC, ...)
Peter Coveney (UCL, CompBioMed, QCi3, ...)
Sir Peter Knight (Imperial, NPL, ...)

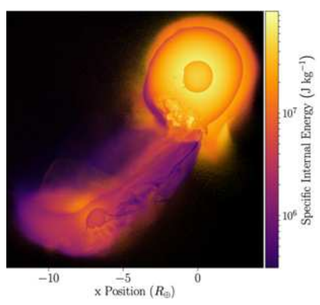

Image from RMP 86:153 (2014)

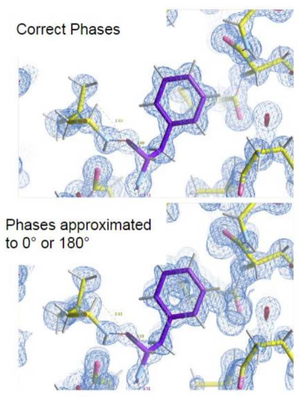

Figure illustrates the difference between a density map using the correct phase angles and when we approximate them to 0^o or 180^o, whichever is closest. This gives an average error of 45^o, over the entire set of reflections.

More projects and collaborations:

Smoothed Particle Hydrodynamics (SPH) – many discrete masses approximate a continuum, often a fluid. Particles move in a Lagrangian manner according to conservation of mass, energy and momentum. Violently deforming and fragmenting material interfaces can be modelled without the special treatments required in mesh-based methods. Collaboration with QCi3 Quantum Tech Hub.

[1D proof-of-concept: arXiv:2006.06719, CPC 294 108909 2024; mutiple time steps arXiv:2503.05393, Phys. Fluids 37 057141 2025] *Figure shows a mid-collision snapshot of a planetary grazing impact using 10^8 SPH particles*

lattice Boltzmann method (LBM) – also widely used for fluid simulation, especially multiphase flows and complex boundaries. Maps naturally to a quantum version of a random walk, with extra qubits to treat the nonlinear relaxation. Collaboration with UKCOMES and the Université Aix-Marseille.

Macromolecular Crystallography (MX) phase problem (CCP4)

Structure solution through diffraction experiments on crystals is central to a wide variety of sciences. The same problem (inverse FT) also arises in radio astronomy (Square Kilometer Array). The experiments record the amplitude but not the phase of the diffracted wave. Quantum computing offers the possibility of a direct solution. Each of the up to 10^8 reflections in a collected experimental diffraction set have a phase angle between 0^o and 360^o when they hit the detector. These angles cannot be measured. However, if they can be approximated to an average error of 45^o or less, then the electron density map for the target molecule can be reconstructed to high accuracy.

October 31, 2025

Engineering and Physical Sciences Research Council
Science and Technology Facilities Council
QCi3 HUB
National Quantum Computing Centre
University of Strathclyde Science