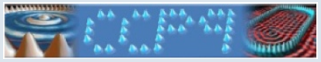
Grand Challenges

The Collaborative Computational Project Number 9: Computational Electronic Structure of Condensed Matter (CCP9)

First principles materials modelling is the keystone of modern technology, allowing us to understand, exploit and design materials with the special properties we need. CCP9 supports materials modelling by maintaining high-performance simulation codes, conducting pioneering theoretical research and by fostering the UK community of material simulation specialists.

The Community



www.ccp9.ac.uk

CCP9 was established in 1980 to advance methods and code development in the UK materials modelling community. Since then, CCP9 has provided a crucial network connecting UK-based research groups in electronic structure, coordinating both research and software engineering activities and organising training in the theory and application of coding. Their collaboration, coordination and community elements have significantly contributed to gaining and maintaining UK leadership in theoretical materials science.

The Challenge

To meet and fulfil the growing demands of a new, multiscale simulation paradigm spanning diverse technology fields

Technology and engineering priorities place huge challenges on the Electronic Structure community as we continue to develop methods for delivering clearer science insight and answers to ever more complicated questions. The main challenges before us are to integrate and fully utilise new approaches to science: **Interoperability with AI**, which will allow us to not only accelerate our codes but also automate their execution and help with analysis of outputs; **Interoperability with Quantum Computing**, which will allow solution to previously unsolvable physics problems; and, **Black-box like precision and reliability** enabling our methods to be deployed without laborious human control. And as our codes scale to use ever larger computational facilities, we must pay serious attention to **Energy efficiency and new architecture exploitation**.

Grand Challenges

The Solution

Interoperability with both AI and quantum computing, energy efficiency and new architecture adoption

AI/LLM technologies will be used to accelerate first principles materials modelling by optimising the selection of specific materials cases and properties for calculation, by automating the preparation of calculation inputs, by accelerating or improving algorithms in the electronic structure codes and, even, by providing new, more efficient approximations for the fundamental theories that our codes implement (eg, approximations for the unsolvable electron-electron correlation problem).

As quantum hardware becomes available with sufficient capability for real calculations, we will develop the algorithms that are needed for their use. Condensed matter physics and computational chemistry areas are the first application areas for this new technology and we expect quantum computers will make possible previously unsolvable problems, or else attain huge efficiency gains, compared with current modelling approaches.

Historically, calculations using electronic structure theory were limited by available resources, codes and level of theory; reproducibility and accuracy were less important than the specific scientific insight afforded by calculations to scientists' specific projects. The expert user (who usually authored the code) was indispensable. CCP9 will adopt a new modelling paradigm where electronic structure calculations will be applied as part of (potentially hugely) complex studies working across scales from the atomic to the gigantic. Numerical and other errors will be understood, quantified and become systematically controllable, allowing our methods to be deployed successfully by AI-enabled non-experts working in widely different topics.

The Outcome

A suite of codes that can be applied routinely by non-experts in complex, AI-enabled workflows

The CCP9 community will build upon its global leadership in electronic structure to provide a suite of codes that can be applied routinely by non-experts in complex, AI-enabled workflows in simulation areas extending well beyond the materials science area. Quantum computing will be added to the CCP9 portfolio of state-of-the-art methods enabling new simulation possibilities.

More Information

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