Grand Challenges

The United Kingdom Car-Parrinello Consortium (UKCP)

Over the next five to ten years, UKCP will enable reliable, efficient and predictive simulations of a wide range of materials systems critical to many of the UK Government's missions including "Make Britain a Clean Energy Superpower"

The Community

www.ukcp.ac.uk

UKCP is one of the longest-running High-End Computing Consortia in the UK. The member groups develop quantum mechanics-based simulation methods at the cutting edge of science and capability computing. These methods are generally applicable with key areas that include electric battery materials, photovoltaics, additive manufacturing, and pharmaceutical design. UKCP leads the development of three UK materials modelling packages and contributes to three others, with dozens of community tools across chemistry, physics, engineering and materials sciences. One of the UK apps supported by the consortium, CASTEP, has over 2000 licensed academic research groups and 1000 industrial sites, across 90 countries. The users of these simulation apps include many experimental research scientists, who use the tools to analyse and interpret experimental data and design new experiments. UK national facilities routinely use UKCP developed software, such as Diamond Light Source, ISIS Neutron and Muon Source, and UK High-Field Solid-State NMR Facility. The large global userbase has been made possible only by sustained investment in research software engineering (RSE) over three decades, which has led to software which is capable of advanced quantum mechanical materials simulations. This software can be run efficiently on machines from laptops to supercomputers, with user-friendly interfaces that enable effective use by non-computational specialists.

The Challenge

Deliver effective simulations for materials research with efficient use of future computing capabilities

The methods and software developed by UKCP are applicable to all four themes of the government's industrial strategy. The challenge is to remain at the forefront of state-of-the-art materials simulation while also making the best use of the computational resources available now and in the future. It is essential to incorporate emerging and fast-moving technologies such as quantum computing and AI in the methods and workflows of the community. New methods, technology and techniques offer the challenge of whole-device simulation, combining software across UK communities, to enable rapid advancement of product design and manufacturing processes.

The Solution

Develop new methods to improve materials software, leverage emerging technology and deliver training

Over the next decade UKCP will:

- Develop advanced new methods and techniques to improve the usability, accuracy and performance of materials software, to extend its scientific capabilities to model new experimental properties.
- Derive and implement rare-event sampling methods, multiscale and multiphysics models, and techniques to model dynamics and disorder in complex systems.
- Work with hardware and software vendors to co-design solutions to the technical challenges faced in materials modelling software development.
- Transform our software modelling tools' performance, by developing new algorithms and using both hardware (e.g. GPUs) and software (AI) acceleration.
- Address the AI and Digital Skills gap: Partner with other consortia and computing facilities to devise and deliver training to support both RSEs and scientific researchers, and "Break Down Barriers to Opportunity" by supporting and encouraging currently under-represented groups.

The Outcome

Guide experimental design, expand time scales of materials simulations and train and nurture next generation of users and developers

UKCP will enable world-leading experimental scientists to guide experiment design, interpret, and even predict results, without the need for them to become computational specialists. They will expand the length- and time-scales of materials simulations by several orders of magnitude, and train and nurture the next generation of expert users and developers. This work will enable reliable, efficient, predictive simulations of a wide range of materials systems, including the discovery and design of new materials for battery electrodes and electrolytes, superconductors, magnetic data storage, medical implants and fusion reactor coolant and containment walls. Their roadmap will: maintain and extend the UK's world-leading research in materials modelling; support a wide range of experimental and computational research and researchers across many disciplines, including physics, chemistry, materials science, engineering, earth sciences and life sciences; enable strategically important work in clean energy, sustainable development and future healthcare; and enhance the digital skills of early-career researchers and the next generation UK workforce.

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More Information

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