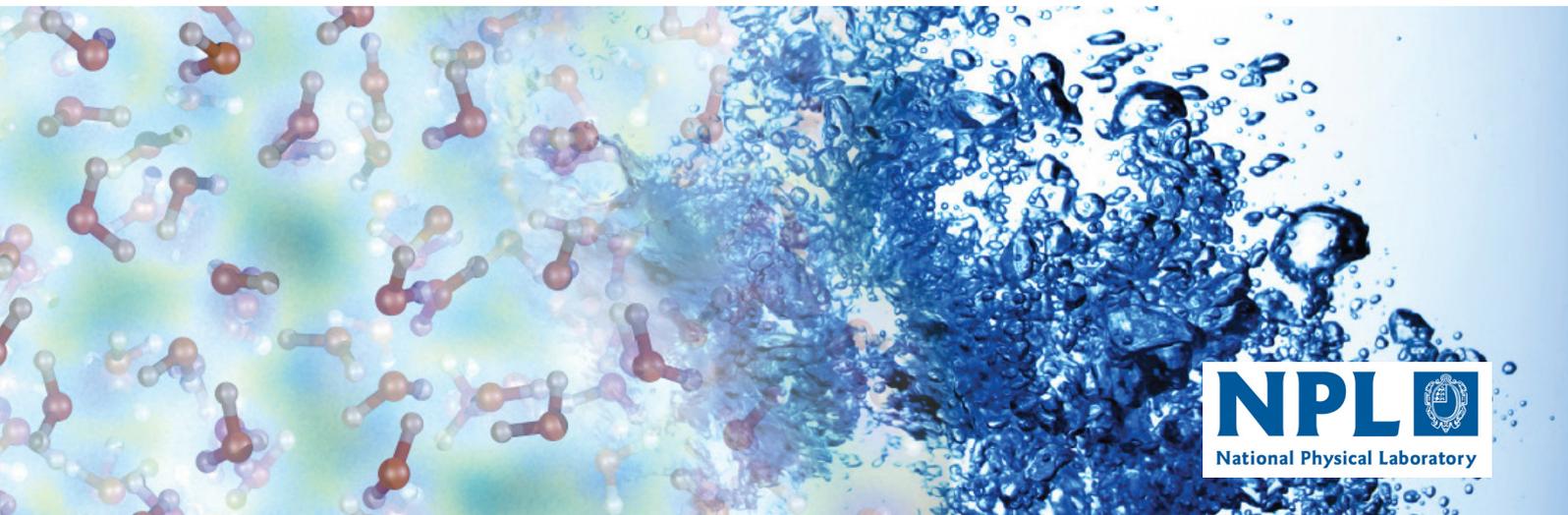


Building next generation materials simulation tools



Hartree Centre
Science & Technology Facilities Council



The UK's National Physical Laboratory (NPL) and international partners are developing a new framework for accurate materials simulation using the STFC Hartree Centre's supercomputing capability.

Challenge

Materials simulation is of growing importance to both industry and the scientific community, as it can be used to save costs in product development by predicting a material's properties where experiments are difficult or uneconomical. At NPL, materials simulation is a key tool used in measurement science to aid data interpretation. Simulations on a fundamental level involve electrons and atoms. Electrons are fast, requiring quantum mechanical description, while atoms are significantly slower and use classical dynamics. Developing complex multiscale methods which combine both quantum and classical parts is one of the biggest challenges in modelling.

Solution

A unique partnership between NPL, IBM Research, the University of Edinburgh and the Hartree Centre is developing a radical new strategy for materials simulation based on a coarse-grained electronic structure that dramatically improves the accuracy of classical simulations at a fraction of the cost of full quantum calculations. The team has now successfully demonstrated the method for a number of test cases using the Hartree Centre's advanced supercomputing facilities, something that was impossible to tackle using any other approach.

Benefits

These innovative new methods help scientists to understand and describe the complex interactions between atoms and molecules, and how they are linked to a material's properties. These links can be exploited in the design of improved processes to handle such materials, providing long-term benefits to both fundamental research organisations and private businesses, initially focussing on biochemical and biophysical fields. The success of this project has the potential to enable and increase the accuracy of materials simulation over a much wider range of conditions and environments. For industry this would mean less physical trials for systems in order to reach the optimum configuration, which increases productivity and reduces wastage of time and resources in the early testing stages.

"NPL's strategy commits us to delivering excellent science to maintain its national and international status as a leading National Measurement Institute. Improving the accuracy of the model predictions is a critical step in developing innovative approaches to measurement challenges. Without the HPC computing capabilities of the Hartree Centre we wouldn't be able to complete our mission."

– Vlad Sokhan, Principal Research Scientist, NPL

Work with us

We collaborate with industrial clients and research partners on projects that create insights and value using high performance computing, big data analytics, simulation and modelling.

By combining our world-class facilities with access to our specialists and computational scientists, we can enable your organisation to produce better outcomes, products and services more quickly and cost-effectively than through conventional R&D workflows.

With our partners we are developing the next generation of supercomputing architectures and software, combining existing best practice with innovation to deliver faster, cooler and more sustainable solutions capable of meeting the challenges of data intensive computing.

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