Supercomputing for materials simulation

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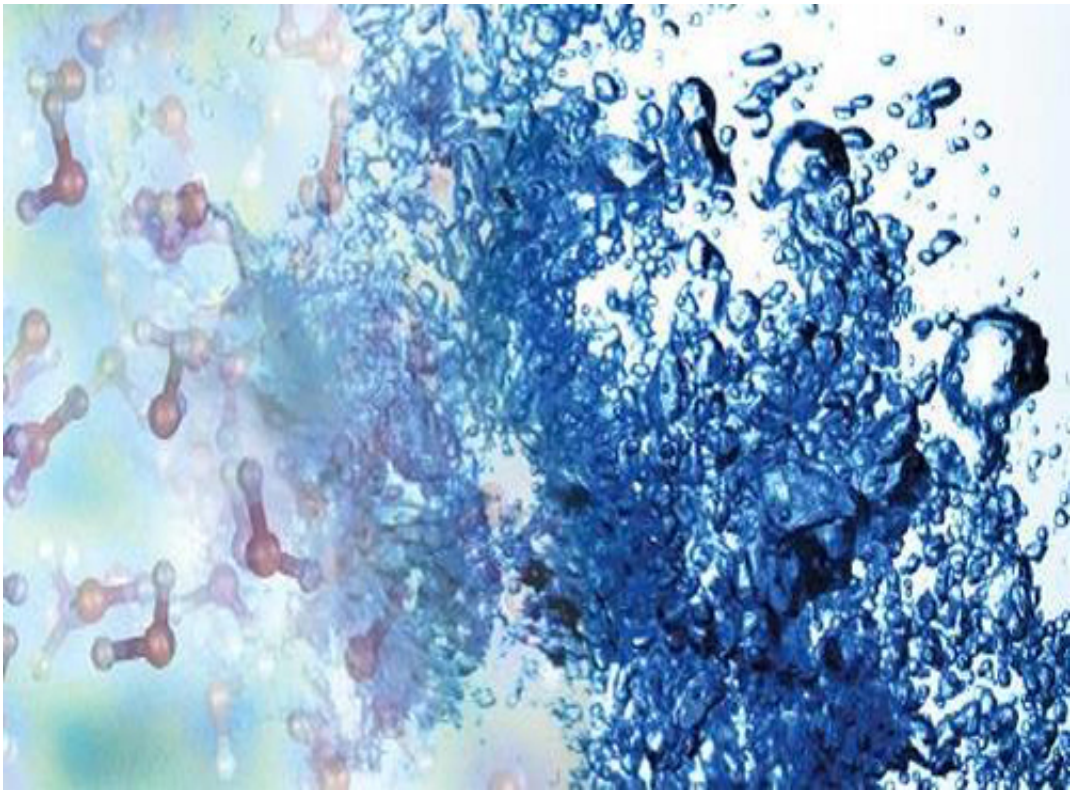

Combining quantum and classical physics is one of the biggest challenges in modelling.

The National Physical Laboratory (NPL) and international partners are using advanced supercomputers to develop a new framework for accurate materials simulation.

The partnership between NPL, IBM Research, the University of Edinburgh and the Hartree Centre for high performance computing aims

to help scientists understand and describe the complex interactions between atoms and molecules, and how they are linked to a material's properties

The Science and Technology Facilities Council (STFC), which operates the Hartree Centre, has published a case study that explains how this work could help save costs in product development by predicting materials properties where experiments are difficult or expensive.

At NPL, materials simulation is a key tool used in measurement science to aid data interpretation. "Improving the accuracy of the model predictions is a critical step in developing innovative approaches to measurement challenges," explains NPL's Vlad Sokhan, who is working on the project.

Simulations on a fundamental level involve electrons and atoms. Electrons are fast, requiring quantum mechanical description, while atoms are significantly slower and described using classical dynamics. Developing complex methods which combine both quantum and classical parts is one of the biggest challenges in modelling.

The partnership has already successfully demonstrated a new method based on a coarse-grained electronic structure for a number of test cases, which would be impossible to tackle using other approaches. The continued success of the project has the potential to enable and increase the accuracy of materials simulation over a much wider range of conditions and environments.

More information: The full case study is available online: www.stfc.ac.uk/3168.aspx

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