Simulations assist more economical oil extraction

Hartree Centre
Science & Technology Facilities Council

Researchers at Lancaster University are using the supercomputing capability of the Hartree Centre to accurately simulate the flow of complex fluids to improve oil extraction techniques.

Challenge

High oil prices, growing demand and few new field discoveries mean that the need to find better oil extraction techniques is increasingly urgent. Within the oil industry, there is great interest in in stabilising flows through oil reservoirs to enhance extraction. However, efficiently modelling oil flow in reservoirs can be complex and time consuming due to the intricate geological environment and high pressures involved, and so these multifaceted calculations require a compute intensive capability. The grand challenge is to accurately simulate the flow of complex fluids through pores with length scales that are more similar to the porous media encountered in real oil fields.

Solution

To simulate the complex fluid at a sub-micron scale, the team first modelled a single molecule dispersed in a small number of water molecules. These atomistic calculations are computationally expensive, meaning they take a great deal of computing power to process, but are necessary to produce atomic-scale parameters that can be used as input for larger, 'meso-scale' molecular dynamic simulations. This approach makes it possible to maintain accuracy when scaling up the calculations, without expending large quantities of unnecessary computational resources. Researchers used a suite of packages developed at the Hartree Centre in their calculations to translate the simulation from atomic-scale (DL_POLY) to meso-scale (DL_MESO). Parameters from the meso-scale were then utilised in continuum models to approximate the flow of oil.

Benefits

Using high performance computing, simulation and exploiting key computational chemistry technologies, the researchers managed to significantly shorten the time taken to carry out the calculations. Access to the optimised parallel architecture at the Hartree Centre was crucial to achieving the sub-micron scale parameters the scientists required. The ability to present unique, leading edge results at a lower R&D expenditure has also greatly improved the competitiveness of the group and this study is significant for the oil industry as it may lead to new strategies to stabilise flows through reservoirs with the subsequent enhancement of oil extraction processes..

"Despite having access to an excellent high performance cluster at Lancaster, we found that the existing capability of the cluster would have resulted in a time frame for our calculations that was far in excess of the time available. The Hartree clusters enabled us to use higher levels of parallelisation and cut down the calculation time considerably."

– Dr Steven Bailey, Research Fellow, Lancaster University

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