Scalable Continuum-to-Molecular Coupling and Embedding Module Developed by HECToR dCSE Team

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HPC experts from ICL and NAG, working under NAG's Computational Science and Engineering (CSE) support service for HECToR, the UK's national academic supercomputing facility, have successfully developed a module which may be used to interface independent applications for molecular and continuum scale simulation, thus enabling highly-scalable multi-physics simulations on HECToR.

The Continuum-to-Molecular Coupling and Embedding (CMCe) module enables distinct computer codes to solve fluid flow problems across a wide range of physical scales on HECToR. In particular, coupling the Direct Numerical Simulation (DNS) code, Transflow, and the Molecular Dynamics (MD) code, StreamMD, has demonstrated good scalability for 1,000 cores on HECToR with a Lennard-Jones system of 3 million molecules.

Commenting on the dCSE project success, *Dr Tamer Zaki of Mechanical Engineering at ICL said: "The idea of the dCSE support is unique, and provides essential support to researchers in various strands of research that rely on high-performance computational science. The dCSE provides an opportunity to interface researchers from different backgrounds with computer scientists from NAG, to demonstrate the importance of software design and optimisation and to engage in new areas of software development that might not be possible via other sources of funding."*

"In our case in particular, we have benefited from the dCSE program in many of the above aspects. We aimed to couple two well-established algorithms that we have developed and scaled up to thousands of cores, but which were simulating completely different physical scales. Via our interaction with developers from NAG, we were able to abstract the problem to a point where our development is not only robust for our particular applications, but sufficiently general that it becomes of value for the wider community of HECToR users and multi-physics researchers. We have also benefited from our interaction with NAG software engineers in aspects of robust development, automatic checks, version tracking and documentation. At the end of the initial phase, we had developed sufficient knowledge transfer from NAG to our group that we were confident that we could guarantee the success of the second phase."

With the newly developed CMCe module, a parallel efficiency of at least 90% can now be achieved with coupled DNS and MD simulations, using several thousands of cores on HECToR.

"The coupler that we developed during our dCSE project has enabled new science. We are now able to simulate any interfacial, micro-scale phenomenon using accurate Molecular-Dynamics simulations, while simultaneously evaluating the macroscopic impact using our continuum solver. We are applying these techniques for studies of wall slip, surface textures and coatings, and constitutive modelling of exotic and complex fluids. We are also collaborating with other groups that are interests in surface effects in tribological applications, and our colleagues from chemical engineering are interested in moving contact line problems. In addition, we anticipate that the coupler which we developed will be adopted by the wider research and HECToR communities for interfacing other applications, where the phenomena of interest require accurate representation of the physics at various scales or from various disciplines."

HECToR

HECToR is managed by EPSRC on behalf of the participating Research Councils with a mission to support capability science and engineering in UK academia. The Cray XE6 supercomputer, located at the University of Edinburgh, is managed by UoE HPCx Ltd. The CSE Support Service is provided by NAG Ltd and ensures users have access to appropriate HPC expertise to effectively exploit advanced supercomputers for their science. A critical feature of the CSE Support Service is the distributed CSE (dCSE) programme which, through lightweight peer review, delivers dedicated performance and scalability projects on specific codes in response to proposals from users. The dCSE programme now consists of over 70 focused projects complementing the traditional HPC user applications support and training also provided by NAG.

The dCSE projects completed so far have delivered outstanding examples of the cost savings and new science that can be enabled through dedicated CSE effort. The CMCe module project reported here adds to these success stories with a successful performance improvement.

Project Background

The objective of this project was to enable massively parallel and highly-scalable simulations for coupled DNS and MD simulations. This would be achieved by developing a CMCe module, to serve as an interface protocol between the large-scale, macroscopic features of a fluid and also the atomic-level behaviour near flow boundaries.

Tamer Zaki of Mechanical Engineering at ICL was the Principal Investigator for the project. Edward Smith and David Trevelyan also of ICL along with Lucian Anton of NAG all contributed to the 12 person-months project, in close collaboration with the NAG CSE team.

Project Results

The newly developed CMCe module allows the DNS (Transflow) and MD (StreamMD) applications to be run in Multiple Program Multiple Data (MPMD) mode. During simulations, data exchange is now performed via calls to the CMCe module from Transflow and StreamMD. This ensures that all scalability characteristics of the individual client (Transflow and StreamMD) applications are retained. Furthermore, this also ensures that any number of MD instances can interface to the DNS (continuum) solver, facilitating "MD farming".

The weak scalability of TransFlow for a test case with 10^6 grid points per MPI task can now achieve 90% parallel efficiency on HECToR and StreamMD with 3.3×10^6 molecules, 94% parallel efficiency. The overall scalability with the CMCe module is therefore excellent for coupled CFD and MD simulations with grid points and molecules in the order of millions, using several thousand of cores on HECToR phase 3.

Currently, plans are underway to host the CMCe coupler library online, in order to help facilitate multi-physics simulations in the wider research community.

Full technical reports on this work can be found at http://www.hector.ac.uk/cse/distributedCSE/reports/transflow01/ and http://www.hector.ac.uk/cse/distributedCSE/reports/transflow02/

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