Scaling of General Purpose, Multi-Phase CFD Code (Fluidity) Improved with NUMA-Aware Memory Access Techniques by HECToR dCSE Team

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An HPC expert from EPCC, working under NAG's Computational Science and Engineering (CSE) support service for HECToR, the UK's national academic supercomputing facility, has speeded up the matrix assembly and matrix solver steps in Fluidity by improving the ordering of the topological and computational meshes. The reordering is achieved by implementing a space-filling curve approach to order the nodes and elements of the mesh in each MPI process to achieve an optimal communication pattern on NUMA (Non-Uniform Memory Access) architectures.

Fluidity was developed by the Applied Modelling and Computation Group (AMCG) at Imperial College. Its focus is ocean modelling. Fluidity is capable of resolving flows simultaneously on global, basin, regional, and process scales, enabling oceanographic research that is not possible with other models. It is an adaptive model that can optimise the number and placement of computational degrees of freedom dynamically through the course of a simulation. The long term aim is the ability to simulate the global circulation and to resolve selected coupled dynamics such as ocean boundary currents, convection plumes, and tidal fronts on the NW European shelf down to a resolution of 1km. Fluidity currently runs on a range of computing platforms, from desktop workstations to HPC platforms. However, the size of problems that can be investigated is limited, especially on systems with NUMA multicore processors, such as HECToR. The purpose of this project is to improve the scaling behaviour of Fluidity by implementing memory access techniques that better exploit the hybrid OpenMP/MPI code within the finite element assembly and solve routines.

Commenting on the dCSE project success, *Dr Jon Hill of the Applied Modelling and Computation Group at ICL said: "This DCSE project successfully implemented mesh renumbering within Fluidity using the space filling curve implementation provided by the Zoltan framework. This can now be applied when a new mesh is read at the outset of a simulation, either in serial or in parallel, and each time the mesh is changed by mesh adaptation. It was verified that the numbering was applied to the mesh correctly. While initial tests indicated that the performance benefit was small, matrix-vector multiplications, for example, showed only a marginal decrease in the number cache-misses. However, now that the renumbering functionally has been added, developers are able to perform more detailed analysis to how to refactor data structures to improve data streaming."*

By implementing improved memory access techniques that better exploit the hybrid OpenMP/MPI code within the finite element assembly and solve routines in Fluidity, improved scalability can now be achieved. This could reduce the kAU footprint of Fluidity by 5% (1,000 kAUs) per year.

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 Fluidity project reported here adds to these success stories with a successful performance improvement.

Project Background

The key objective of this project was to improve the ordering of topological and computational meshes in Fluidity by extending its decomposition method, and adding mesh renumbering to the central trunk code. Correct functionality would be checked with new tests added to the existing suite of 22,000 unit and regression tests while also profiling NUMA performance.

Jon Hill of the Applied Modelling and Computation Group at ICL was the Principal Investigator for the project. Mark Filipiak of EPCC carried out the 6 person-month project, in close collaboration with the NAG CSE team.

Project Results

A Hilbert space-filling curve (HSFC) method was implemented to order the nodes and elements of the mesh in each MPI process. This was achieved by using the HSFC from the Zoltan library, which is already used by Fluidity for mesh decomposition and load balancing across MPI processes. The use of Zoltan had been previously implemented in Fluidity as part of an earlier dCSE project.

A 3D backward-facing step simulation with 1,000,000 finite element nodes (grid points) was used as a representative test case and this demonstrated that the new mesh reordering gives a 5% speed-up overall. However, the performance varies with thread placement over the UMA regions within the HECToR node.

Hilbert space-filling curve reordering could also be applied to other finite element codes running on HECToR to give a similar speed-up.

A full technical report on this work can be found at http://www.hector.ac.uk/cse/distributedcse/reports/fluidity-decomp/

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