BOFFS High-Order CFD Solver Developed for Improved Scalability on Many-Core Architectures by HECToR dCSE Team

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HPC experts from NAG, working under NAG's Computational Science and Engineering (CSE) support service for HECToR, the UK's national academic supercomputing facility, have successfully improved the hybrid OpenMP-MPI parallel code, BOFFS, which is used to perform high resolution Large eddy simulation (LES) models.

The Block Overset Fast Flow Solver (BOFFS) is a high-order CFD code which is used on overset, structured grids to perform LES of turbulent flows, mainly for turbomachinery applications.

This dCSE project has enabled LES to be performed on HECToR with BOFFS for grids with more than 100 million points and hundreds of blocks. This was achieved by developing the existing hybrid OpenMP-MPI parallelism within BOFFS to allow the code to fully utilise the thousands of processing cores available on HECToR.

Commenting on the dCSE project success, *Dr Richard Jefferson-Loveday of the University of Cambridge said: "We have found the dCSE work performed on our CFD code 'BOFFS' extremely beneficial. It has enabled us to simulate a large range of turbine flows including rim-seals, labyrinth seals and transitional flows in LPTs. The roughness work performed is of vital importance to UK industry and offers potential for direct design improvements through the control of surface finish and insights on blade replacement schedules. Future work includes using the code to improve our understanding of the effects of temperature, flight speed and complex geometry on jet aeroacoustics. Around 50,000 kAU's have been assigned for use with BOFFS in gas turbine related projects. The support provided by the dCSE team has been excellent throughout the duration of the project and beyond."*

BOFFS can now utilise up to 8 threads per MPI task enabling up to a 1.5 times speedup to be achieved compared with the original code. This project has enabled BOFFS to utilise HECToR more efficiently, meaning that future LES of turbulent flows on grids with more than 100 million points (and with hundreds of blocks) are now a possibility for BOFFS.

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

Project Background

The objectives of this dCSE project were to enable more realistic turnaround times for BOFFS on grids with more than 100 million points (hundreds of blocks), by improving code efficiency in 3 parts: the MPI used for the inter block data transfers, the memory utilisation and the OpenMP for the intra block computations.

Dr Richard Jefferson-Loveday from the Department of Engineering at the University of Cambridge was the Principal Investigator for the dCSE project. Lucian Anton, Ning Li and Phil Ridley of NAG carried out the 4 person-month project, in close collaboration with the NAG CSE team.

Project Results

For the inter block data transfers, an asynchronous method to transfer data between blocks was implemented with MPI. The transfers are now performed in a third of the original time and furthermore, grids with more complex block structures can be studied. Code was also re-factored to remove large static arrays. Finally, the OpenMP sections for the intra block computations in the Tri-Diagonal Matrix Solver (TDMA) were improved by implementing a red-black decomposition.

The updated BOFFS is now scalable for up to 8 threads per MPI task. Reasonable performance for up to 32 threads can be achieved for certain problem sizes. A 1.5 times speedup can now be achieved for a 12 million grid point, 4 or 32 block test case running on HECToR.

The primary application of BOFFS is in the area of turbomachinery and it is used mainly within group at Cambridge, Warwick and Cranfield Universities, e.g. for simulations of a Boeing Fan in EPSRC project EP/I010440/1. HECToR use of BOFFS has so far consumed around 50,000 kAUs for investigation of the aerodynamics and aeroacoustics of complex geometry hot jets through EPSRC research grants EP/G027633/1, EP/G069581/1, EP/F005954/1, EP/I017771/1.

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

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