Performance of Turbulent Fluid Flow Simulations (Incompact3D) Improved by Factor of 6x 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 implemented scientifically valuable new functionality and substantial performance improvements in the Incompact3D application.

Incompact3D is a CFD application for direct and large-eddy simulations (DNS/LES) of incompressible flows. One recent application of Incompact3D is to complement experimental results from wind tunnel measurements for studies of turbulence generated by multi-scale/fractal objects. This class of new flow concepts is offering possibilities for brand-new solutions useful in industrial mixers, silent air-brakes, new ventilation and combustion devices. To resolve the turbulent eddies associated with the smallest scale wind tunnel measurements, very high resolution multi-scale flow simulations are required, which requires powerful supercomputing resources.

Commenting on the project success, Christos Vassilicos (the Principal Investigator) said "*In order to better understand the origins of the original properties of multi-scale objects, it was necessary to undertake high-fidelity simulations of such unique complex flows. Because of the complexity of the flow configuration, these simulations require hundreds of millions of mesh points and thus it was almost impossible two years ago to perform the numerical modelling. The new version of the code is a blessing as it will speed up our research and will allow us to do accurate comparisons with experiments*."

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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 XT supercomputers, located at the University of Edinburgh, are 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 50 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 Incompact3D project reported here adds to these success stories with a major performance improvement.

Project Background

The objectives of this dCSE project were to enable Incompact3d to run on thousands of processor cores in order to reduce the wall-clock time of a simulation and also to enable it to run bigger simulations with as much complexity as possible to match real-life experiments. This was to be achieved by updating the original domain decomposition strategy from a 1D (slab) to a 2D (pencil) domain decomposition for the FFTs and improving the global transpositions with a shared memory approach to the MPI_Alltoallv(s). Additionally, the vector version of Incompact3D was to be enhanced with OpenMP, the MPI parallel and vector versions of Incompact3D were to be merged into a more portable version of the code.

Christos Vassilicos of Imperial College London was the Principal Investigator on the project. Ning Li of NAG carried out the 16 person-month project in collaboration with the NAG CSE team and the Incompact3D developers. Nearly 70 million AUs (allocation units) have been used on HECToR to run Incompact3D simulations so far.

Project Results

The original Incompact3D employed a 1D slab data decomposition. This limited its application to large-scale simulations due to the scalability constraints, hindering productive scientific studies. A typical simulation involving a 2048*515*512 mesh could only utilise up to 512 cores. On HECToR Phase 1, this would mean a runtime of 25 days (wall-clock time). This size of mesh can now utilise 8000 cores efficiently, with a run time of around 3.75 days (wall-clock time) which is over 6x faster. Furthermore, meshes for new high resolution turbulence mixing and flow control simulations which use up to 4096*4096*4096 grid points, can now utilise as many as 16384 Phase 2b cores.

The decomposition framework developed in this dCSE, 2DECOMP&FFT, is available to all HECToR users for scientific applications that may require upgraded distributed FFT calculations, e.g. combustion, ocean modelling and compressible CFD. More generally, it has been submitted to the Open Petascale Library project under an open-source licence. It has already been used in several other projects (including dCSE).

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

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