Performance and Capability of Turbulence Flow Solvers Improved by HECToR dCSE Team

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An HPC expert from NAG, working under NAG's Computational Science and Engineering (CSE) support service for HECToR, the UK's national academic supercomputing facility, has successfully improved the scalability and capability of three CFD codes which are used to conduct state-of-the-art turbulence studies. Incompact3D, is an incompressible Navier-Stokes solver and its sister codes: Compact3D and QuasiCompact3D, are used for compressible flow simulations.

The aims of this project were firstly to enable the efficient parallel simulation of large-scale compressible turbulent flows, and secondly to enable the embedding of explicit numerical schemes within the framework of a spatially implicit code. This would enable efficient utilisation of more cores on HECToR for turbulence simulations and also enable studies for a wider range of problems, e.g. particle-turbulence interaction. Following this work, Incompact3D now regularly uses 4,000-16,000 cores on HECToR for production runs with a representative parallel efficiency of 80%.

Commenting on the dCSE project success, Dr Sylvain Laizet of ICL said: ''I am currently undertaking Direct Numerical Simulations with Incompact3d. The work is about turbulent plumes in a channel flow configuration with a tilted ramp. In this numerical work, the mixing of fresh water with salty water in a channel flow configuration along with particle settling processes is investigated. In particular, the influence of a tilted ramp inside the computational domain that is modelled using an Immersed Boundary method is studied in order to reproduce real life configurations. 3D interpolations are needed to prescribe the correct boundary conditions on the ramp and it can only be done with the halo-cell communication code newly introduced. The idea is to use an explicit stencil-based method for 3D interpolations to correctly impose boundary conditions for the velocity, for the salinity and for the particles (while the rest of the code still uses an implicit compact finite difference method)."

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"Concerning Compact3d, some simulations of a 3D temporal mixing layer at relatively high Reynolds numbers are currently running in the framework of a collaboration between the University of Poitiers in France and Imperial College (PRACE project for acoustic predictions). So far, Compact3d has only been run on a single node. However, the new version of the code will allow ground breaking progress in compressible flows with configurations very close to experiments. We are also planning to combine an Immersed Boundary Method with Compact3d, in a same way as Incompact3d, in order to put a solid body inside the computational domain. The aim is to investigate grid-generated turbulence for compressible flows."

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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 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 Incompact3D and its sister codes reported here adds to these success stories with a successful performance improvement.

Project Background

There were two aims of this dCSE project: to enable more efficient parallel simulation of large-scale compressible turbulent flows on HECToR; and to develop the facility to perform studies for a wider range of problems, e.g. particle-turbulence interaction.

Professor Christos Vassilicos of the Faculty of the Department of Aeronautics at ICL was the Principal Investigator for the project. Ning Li of NAG carried out the 6 person-month project, in close collaboration with the NAG CSE team.

Project Results

Parallel implementations of Compact3D and QuasiCompact3D were developed by using the 2DECOMP&FFT framework which is an open-source package and is now used by scientists worldwide. Furthermore, a general communication routine was implemented in 2DECOMP&FFT to enable halo-cell communication between neighbouring blocks within the framework of transpose-based parallel codes.

Compact3D and QuasiCompact3D were developed with the help of the NAG Fortran Compiler version 5.3. In particular, the reuse of key subroutines across the codes was employed to improve maintainability, along with the use modern Fortran features. Scalability on HECToR Phase 3 was demonstrated using a test case of 151×203×151 and a parallel efficiency of 80% is now achievable on larger problems using thousands of cores.

As a result of this project, Incompact3D now regularly uses more than 10,000 cores on HECToR for production runs. Furthermore, the new communication code is being used to implement key algorithms within Incompact3D, such as the 3D interpolations required by the Immersed Boundary method to prescribe boundary conditions on the fluid-solid interface, and similar interpolation schemes required to implement particle tracking..

A full technical report on this work can be found at http://www.hector.ac.uk/cse/distributedcse/reports/incompact3d02/

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