Performance and Capability of Turbulence Flow Solver, Incompact3D Further 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 introduced the overlap of communication and computation capability in a CFD code which is used to conduct state-of-the-art turbulence studies.

Incompact3D is an in-house computational fluid dynamics code used by the Turbulence, Mixing and Flow Control group at Imperial College and its academic collaborators to conduct state-of-the-art turbulence studies. The work follows on from two previously successful dCSE Incompact3D projects that significantly improved the scalability of the code, enabling it to use more than 10,000 cores on HECToR for production runs. However, as more cores are used, time spent communicating between nodes becomes more prominent, indicating that there is room for further development.

The objective of this project was to reduce the time taken in all-to-all communications, which is particularly important, when utilising large core counts on HECToR. This was accomplished by further developing the 2D decomposition and Fast Fourier Transform library, 2DECOMP&FFT to perform computations that overlap across-node communications.

Commenting on the dCSE project success, *Dr Sylvain Laizet of ICL said: "When the recent update of HECToR increased the number of cores per processor to 32, we observed that the communication within a processor could be a limiting factor for running large simulations with Incompact3D. With dCSE software support, further development of the code reduced the time taken by the all-to-all communications in Incompact3D by about 15%. By using a library solution, 2DECOMP&FFT, there was little impact on end users. Our code Incompact3D is now available as an open source code through a Google project with about 75 new users worldwide since November 2012, opening many possible collaborations within the UK. These three successful dCSE projects related to Incompact3D now enable us to perform highly accurate large scale simulations in conjunction with our experimental results that form a central component of our research effort. As such, the added value is critical."*

A simulation using multiple independent FFTs demonstrated a performance gain of up to 15%.

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 Incompact3D reported here adds to these success stories with a successful performance improvement.

Project Background

One of the objectives of this dCSE project was to develop a flexible data layout in the decomposition and fast Fourier transform library, 2DECOMP&FFT. This enables wider support for legacy applications and should also improve the performance of some numerical algorithms due to memory pattern changes that could offer more efficient cache usage. Most importantly, the flexible data layout facilitates fine-grain partitioning and reduces the time spent copying data unnecessarily.

Another objective was to create an alternative FFT code for Incompact3D by developing communications that efficiently overlap computation. This would enable multiple independent FFTs to be performed in one library call. Similar efforts would be made to facilitate overlapping computation with communication in various other algorithms.

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 5 person-month project, in close collaboration with the NAG CSE team.

Project Results

Overlapping computation with communication in the 2DECOMP&FFT library achieved a performance gain of up to 15%, enabling multiple independent FFTs to run in a single library call. This work has also made Incompact3D ready for future developments to enable new studies in the simulation of Turbulent Flows.

Software developed from this dCSE project has been released to the general scientific community. The modified 2DECOMP&FFT library was released in October 2012, and the entire CFD code Incompact3D was open-sourced as a Google Project (http://code.google.com/p/incompact3d/) in November 2012.

A full technical report on this work can be found at http://www.hector.ac.uk/cse/distributedcse/reports/incompact3d03/

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