Scalability and Efficiency of Navier-Stokes Codes Improved by HECToR dCSE Team

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An HPC expert from the University of Southampton, 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 efficiency of two key codes which are used to solve the Navier-Stokes (N-S) equations using pseudospectral methods. SWT has been used for the direct numerical simulation of turbulent flow in an infinite plane channel and turbulent Couette-Poiseuille flow. SS3F solves the incompressible N-S equations in the Boussinesq approximation using a 3D-Fourier representation and is predominantly used to simulate the dynamics of vortices in stratified flow. Both codes are used within the UK Turbulence Consortium.

By employing a pseudospectral method, the nonlinear advective terms of the N-S equations must be evaluated in real space such that the necessary transformation to and from wave space is carried out in slices (data decompositions). Before this work, both SWT and SS3F used a 1-D parallel data decomposition which becomes restrictive at higher numbers of processors since the decomposition is limited by the number of collocation points in one of the three spatial dimensions. By implementing better data decompositions in both codes, their strong scalability has been substantially improved: SS3F now scales to over 12000 cores and SWT to 8192 cores for a representative fixed problem size.

Commenting on the dCSE project success, *Professor Gary Coleman of the University of Southampton said: 'This work allows us to make efficient use of current and future HEC resources, and consider problems and regimes that otherwise would have gone unaddressed.'*

> Scientists are able to use the improved SWT and SS3F codes to study turbulent flows with higher Reynolds numbers.

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 SWT / SS3F project reported here adds to these success stories with a successful performance improvement.

Project Background

The aim of this dCSE project was to remove the limit on parallel scalability which had been reached on HECToR with both SWT and SS3F, this was achieved by improving their parallel FFT implementations. In particular, FFTW3 would be used along with a 2-D domain decomposition from the 2DECOMP&FFT library of FFT routines.

Gary Coleman of the Faculty of Engineering and the Environment at the University of Southampton was the Principal Investigator for the project. Roderick Johnstone also at the University of Southampton carried out the 6 person-month project, in close collaboration with the NAG CSE team.

Project Results

Efficiency was improved by just converting the FFT routines to use FFTW3. A 53% reduction in time taken to solution was achieved, for SS3F running a representative 3072×325×1024 mode problem. By updating the 1-D Chebyshev transform used in SWT, a 10^8 mode problem shows an approximate 51% reduction per time step and a 55% reduction for 10^9 modes.

Furthermore, by implementing a parallel 3-D FFT (for SS3F) and 2-D-FFT / 1-D-Chebyshev transforms (for SWT) using the parallel transpose routines of the 2DECOMP&FFT library, scalability for both SS3F and SWT has been improved by over 10 times for representative fixed problem sizes. This approach has enabled test problems of size 10^8 modes to scale to over 8192 cores with SWT; SS3F now scales to 12000 cores, for a problem size of order 10^9 modes.

The test cases used were real simulations, near the limits of the capabilities of the original codes; greater improvements would be expected for more challenging problems, which can only be addressed - if using the original 1-D domain decomposition - by a significant reduction in the core count per node.

As a result of this project, both codes now require – for current scientific work - about half as many kAUs to do the same work on the same number of cores; for SWT, a reduction of 34% could still be achieved while also reducing wall clock time to solution by a factor of 30.

A full technical report on this work can be found at http://www.hector.ac.uk/cse/distributedcse/reports/ss3f-swt/

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