Computational Fluid Dynamics Solver Code_Saturne Ported and Enhanced by HECToR dCSE Team

Zhi Shang, Charles Moulinec, David R. Emerson, Xiaojun Gu, Science and Technology Facilities Council (STFC)
HECToR CSE Team, Numerical Algorithms Group Ltd (NAG)

HPC experts from STFC, working under NAG's Computational Science and Engineering (CSE) support service for HECToR, the UK's national academic supercomputing facility, have ported and optimised the Computational Fluid Dynamics (CFD) application Code_Saturne for massively parallel architectures.

The Computational Fluid Dynamics (CFD) software, Code_Saturne, has been under development since 1997 by EDF. The software is based on a computational method that applies three-dimensional meshes over any type of grid structure, which enables Code_Saturne to simulate fluid flows over highly complex geometries, such as a submarine or an airport tower. It was designed as a parallel code that partitions the data over a mesh to produce the input files for the solver. Once the simulation is complete, the output is converted into files readable by visualization software. Since 2007, Code_Saturne has been open-source.

Commenting on the dCSE project success, *Dr Alistair Revell of the School of Mechanical, Aerospace and Civil Engineering at the University of Manchester said "The work completed in the framework of this project has been highly successful and has had a very significant impact on the widespread usage of Code_Saturne within our research group at the University of Manchester. Substantial improvements have been introduced across a range of items; the overall scalability, I/O performance, parallelisation of pre/post processing stages, and domain decomposition tools. All of these features combined have enabled a step-change in the scale and depth of our computational turbulence research via more efficient usage of HECToR, which has directly benefitted the work undertaken in a number of other research projects."*

Scientists are now able to perform full Computational Fluid Dynamics simulations with Code_Saturne on HECToR enabling a step-change in the scale and depth of computational turbulence research.

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

Project Background

The objectives of this dCSE project were to port the open source package Code_Saturne to HECToR and to improve the pre/post-processing to enable efficient scalability up to 8192 processors on HECToR Phase 2a (Cray XT4) and furthermore enable efficient use of Code_Saturne on the many-core architecture of the current HECToR Phase 3 (Cray XE6). A second objective was to evaluate various open-source mesh partitioning software packages to determine which ones provided the most optimal load balancing and efficient communications that also minimised the memory requirements and data partitioning time.

Project Results

Two widely used open-source mesh partitioning packages were tested for efficiency with Code_Saturne. To perform the 121M tetrahedral element simulation using Code_Saturne, the partition obtained using Metis consistently provided the best decomposition and required the least amount of wall-clock time for the simulation. However, memory constraints varied greatly with each package. For example, the other package, PT-Scotch, was able to generate mesh partitions in parallel up to 131072 domains while using only 16 cores. ParMetis, required a minimum of 512 cores to create the 131072 domains. An analysis of the metrics gathered suggested that the larger number of cores required by ParMetis resulted in a partition but with poor load balancing. In practice, however, the simulation run time did not reflect this observation and, for up to 1024 cores, ParMetis produced the lower time to solution. Above 1024 cores, and up to 8192 cores, the sequential version of Metis showed the best speed-up. For 2048 and 4096 cores, PT-Scotch provided a better performance than ParMetis.

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

For more information contact: HECToR CSE Team
The Numerical Algorithms Group Ltd, Wilkinson House, Jordan Hill Road, Oxford, OX2 8DR, United Kingdom
Telephone: 01865 511 245 Email: hector-cse@nag.co.uk Web: http://www.hector.ac.uk/cse/