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Performance of Magnetic Plasma Turbulence Modelling Code (GS2) Enhanced by HECToR dCSE Team

Colin Roach, Culham Centre for Fusion Energy
Adrian Jackson, Edinburgh Parallel Computing Centre (EPCC)
HECToR CSE Team, Numerical Algorithms Group Ltd (NAG)

An HPC expert from EPCC, working under NAG's Computational Science and Engineering (CSE) support service for HECToR, the UK's national academic supercomputing facility, has substantially improved the parallel implementation of the magnetised plasma turbulence simulation code, GS2, reducing the code's overall run time by up to 20%. GS2 is used to solve the gyrokinetic equations for perturbed distribution functions for all the particle species in a plasma together with Maxwell's equations for the turbulent electric and magnetic fields. It is typically used to assess the microstability of plasmas produced in the laboratory and to calculate key properties of the turbulence which results from instabilities.

Parallel simulations to study low-frequency turbulence in magnetised plasma generally involve FFT calculations along with associated data copying and MPI communications. This work has optimised the transformation of data between the linear and non-linear parts of the code. By implementing a more efficicient approach for the indirect addressing used for the data copying functionality, performance has been improved. Furthermore, an improved 'unbalanced' data decomposition has been developed which provides more flexibility to users by allowing them to select the process count that matches the exact simulation, resources, and system they are using. GS2 can now be used efficiently on HECToR with 2048 cores with a representative reduction in overall runtime time of 17-20%.

Commenting on the dCSE project success, *Dr Colin Roach of the Culham Centre for Fusion Energy said: 'The need to redistribute very large 5-D data arrays is one of the main challenges limiting the maximum practical number of cores that can be used for gyrokinetic simulations. This collaborative dCSE project has allowed us to drill deeply into the innards of the open-source GS2 code, and to make impressive improvements in the code performance at both low and high core counts. GS2 has been around for some years, and these improvements exceeded my expectations. Furthermore, the project has also exposed ideas of very useful improvements that we could make in the future. The outcomes from this project will be of direct benefit to the wide user base of GS2. We are now exploiting this enhanced version of the code to make more efficient use of HECToR in scientific projects, where we are exploring the losses of heat and particles due to electron and ion driven turbulence in tokamak plasmas.'*

The enhanced GS2 code can now be used more efficiently on HECToR to study high-fidelity simulations of turbulence in magnetised plasmas.

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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 GS2 project reported here adds to these success stories with a successful performance improvement.

Project Background

The primary aim of this dCSE project was to improve the performance of the local data copying associated with the data transform between the linear and non-linear calculations, enabling faster computation by reducing the use of indirect addressing. However, during the project it emerged that the data decomposition required by the non-linear calculations could be improved significantly to use resources more efficiently by implementing an unbalanced decomposition.

Performance of the local data copying for all process counts was improved by around 40-50%, by replacing the costly indirect addressing with direct access mechanisms. Introducing the unbalanced data decomposition improves overall performance at higher core counts and allows a more intelligent allocation of resource that is specified by the problem, rather than by the hardware.

Colin Roach of the Culham Centre for Fusion Energy was the Principal Investigator for the project. Adrian Jackson of EPCC carried out the 6 person-month project, in close collaboration with the NAG CSE team.

Project Results

Improved local data copying routines and a better parallel data decomposition method for GS2 have improved performance on HECToR. A reduction in the overall runtime of the code by up to 17% has been achieved for a representative benchmark. In particular with 512 cores on HECToR phase 3, an overall reduction in run time of 7% may be achieved, on 1536 cores the overall reduction is 17%, and with 2048 cores the overall reduction is nearly 20%.

Use of GS2, along with sister codes Trinity and AstroGK has so far consumed over 100,000 KAUs on HECToR from use within the UK plasma physics community. This work will enable a considerable saving of kAUs.

A full technical report on this work can be found at http://www.hector.ac.uk/cse/distributedcse/reports/GS202/

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/