Magnetic Plasma Turbulence Modelling Code (GS2) Given FFT Upgrade & Performance Analysis by HECToR dCSE Team

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HPC experts from EPCC, working under NAG's Computational Science and Engineering (CSE) support service for HECToR, the UK's national academic supercomputing facility, have upgraded the FFT interfaces and undertaken an in-depth performance analysis of the GS2 code used to simulate micro-turbulence within magnetised fusion plasmas. The work revealed that exploitation of SSE instructions for distributed FFTs gave minimal benefit and identified potentially significant performance optimisations.

Modelling fusion plasmas using high performance computing is a key tool to further our theoretical understanding of confining the fusion plasma inside magnetic fields, working towards the goal of producing energy inexpensively from nuclear fusion. Commenting on the dCSE project success, Colin Roach (the Principal Investigator) said "*GS2 is a leading edge gyrokinetic code, and it resolves, in 5-D, fine scale fluctuations in magnetically confined plasmas. Such calculations are extremely demanding, and are yielding insights into the basic turbulent processes that affect the performance of fusion experiments. The dCSE experts have delivered a new parallel interface from GS2 to FFTW3, and performed extensive performance studies. We were surprised, and disappointed, to find that FFTW3 did not deliver the expected performance improvements, but overall this project has been extremely valuable for GS2, and we are delighted with the outcome. GS2 now has a more robust platform for the future, and has identified clear directions for development efforts that ought to deliver significant performance enhancements.*"

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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 XT supercomputers, located at the University of Edinburgh, are 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 50 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 code enhancement and performance analysis.

Project Background

GS2 makes extensive use of fast Fourier transforms in two of its dimensions, via the legacy package, FFTW2. The more active development version of this library, FFTW3, exploits SSE instructions that are available on modern processors. This goal of this dCSE project was to upgrade to FFTW3, which was expected to deliver a substantial performance.

Colin Roach of the Culham Centre for Fusion Energy (CCFE) was the Principal Investigator on the project. Joachim Hein and Xu Guo of EPCC at the University of Edinburgh carried out the 6 person-month project in collaboration with the NAG CSE team and the GS2 users and developers.

The Multiscale Modelling of Magnetised Plasma Turbulence project has an allocation of 75 million AUs (allocation units) on HECToR, representing substantial computing resource.

Project Results

The dCSE project has re-engineered GS2 to add the option of using FFTW3. Following a detailed analysis of the call tree of GS2 the transformation routines have been re-implemented using FFTW3. However, FFTW3's exploitation of SSE instructions has not improved GS2's performance. At the outset of the project it was expected that moving GS2 onto FFTW3 would reduce the time spent on the FFTs. This is because FFTW3 can utilise the SSE instructions of the Opteron processors deployed on the HECToR system, while FFTW2 cannot. Detailed analysis has showed that for the FFT calls relevant for GS2, the benefits from the SSE instructions are at best minimal. This was unexpected and should be of general interest to the HECToR user community. Our detailed analysis has shown that there is little benefit from the SSE even when using smaller problems to make the problem fit into cache or when placing only a single core of the processors to give the compute task more memory bandwidth and level 3 cache.

In addition, other significant GS2 performance issues have been identified where further optimisation should create significant performance gains, in particular, the extensive use of indirect addressing, which cannot be optimised by the compiler. Initial studies show that a clean well-engineered solution to this problem would be very worthwhile in performance terms.

The Multiscale Modelling of Magnetised Plasma Turbulence project has already resulted in seven publications.

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

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