# Step Change in Turbulent Combustion Simulation Code (DSTAR) Enabled 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 enhanced the DSTAR multiphase reactive flow simulation package, improving its scaling efficiency by 50%. Other improvements have made the application's input and output (I/O) more efficient, and improved the structure of the code. The result is an application which can be run efficiently on a vastly larger number of processors, enabling scientists to study more complicated systems (for example, those which incorporate more realistic chemical reaction mechanisms) within their existing compute budgets.

Scientists are able to use the new version of DSTAR to study more complicated systems, enabling the solution of problems that correspond more closely to reality.

The project was focussed on three enhancements: (i) improving the scalability of DSTAR by incorporating a 2D domain decomposition scheme, (ii) optimising the I/O operations for monitoring the evolutionary physical quantities in the simulation, and (iii) refactoring the legacy Fortran 77 code. Commenting on the dCSE project, Prof Kai Luo of the School of Engineering and the Environment at the University of Southampton said: *"This dCSE project has transformed DSTAR by incorporating state of the art parallel programming techniques for multi-core architecture. It prepares DSTAR well for the next generation of massively parallel computers in the UK running at petaflops. The new DSTAR code is able to exploit multi-core HPC architectures and run jobs efficiently on a vastly larger number of processes. This allows the code to make use of much more computing power than before and solve more complex problems. For example, more realistic chemical mechanisms can now be simulated. As a result, combustion simulation will be more accurate or combustion of more types of fuels can be explored."*

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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 60 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 DSTAR project reported here adds to these success stories with the development of an enhanced version of the application.

## Project Background

DSTAR is a code which simulates multiphase reactive flows by solving the complete Navier-Stokes equations, together with conservation equations for energy and chemical species.

Modules for both direct numerical simulation and large eddy simulation have been developed for high-fidelity simulation of turbulence, aeroacoustics, turbulent combustion, multiphase turbulent flow and combustion. DSTAR incorporates highly accurate numerical techniques such as 6th-order spatial discretisation, non-reflecting boundary conditions and low-storage Runge-Kutta explicit time-advancement..

The parallel computation in DSTAR currently uses a Cartesian grid which is partitioned along a single dimension; this dCSE project was aimed at replacing this with a 2D domain decomposition in order to improve the scalability of the application. Another aim of the project was the optimisation of the I/O operations which are used for monitoring the progress of the calculation, and for restart data. Finally, the legacy Fortran 77 code was to be updated to use the modern constructs associated with the successors to that language.

Kai Luo of the School of Engineering and the Environment at the University of Southampton was the Principal Investigator for the project. Lucian Anton, one of NAG's HPC experts, carried out the 6 person-month project, in close collaboration with the NAG CSE team.

DSTAR is currently being used on two HECToR projects with an allocation of 258,800 kAUs (thousands of allocation units); the application for a third project using DSTAR is currently being processed.

## Project Results

A 2D domain decomposition was implemented using the 2DECOMP&FFT library. The new code was tested using two cubic grids of size 768 and 1536, with up to 18,432 MPI tasks; comparison with the old code showed a scaling efficiency of around 50%. In addition, a Mixed Mode programming model was prototyped, which gave better scalability, but resulted in a more complicated source code.

DSTAR uses ASCII I/O for progress data, and binary for restart data. The monitoring I/O is now performed by a dedicated process (previously, many processes would write their local data). An MPI-IO approach to writing the restart data was also implemented, but it was determined that the original method (each process writing its local data) was still faster.

The Fortran 77 source code was re-factored and the main subroutines were rewritten as Fortran MODULES. Where subroutines made poor usage of cache memory utilisation, nested loops were reordered and any redundant IF THEN blocks were also removed, giving performance speedup of around 20%.

Following the conclusion of this dCSE project, DSTAR can handle around 50 times more MPI tasks and grid points than previously. The new version of the code has been made available to all users.

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

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