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Large-Scale Simulations of Turbulence Using Discontinuous Spectral Element Method

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Abstract : Turbulence can be observed in a variety fluid motions in nature and industrial applications. Recent investment in high-speed aircraft and propulsion systems has revitalized fundamental research on turbulent flows. In these systems, capturing chaotic fluid structures with different length and time scales is accomplished through the Direct Numerical Simulation (DNS) approach since it accurately simulates flows down to smallest dissipative scales, i.e., Kolmogorov's scales. The discontinuous spectral element method (DSEM) is a high-order technique that uses spectral functions for approximating the solution. The DSEM code has been developed by our research group over the course of more than two decades. Recently, the code has been improved to run large cases in the order of billions of solution points. Running big simulations requires a considerable amount of RAM. Therefore, the DSEM code must be highly parallelized and able to start on multiple computational nodes on an HPC cluster with distributed memory. However, some pre-processing procedures, such as determining global element information, creating a global face list, and assigning global partitioning and element connection information of the domain for communication, must be done sequentially with a single processing core. A separate code has been written to perform the pre-processing procedures on a local machine. It stores the minimum amount of information that is required for the DSEM code to start in parallel, extracted from the mesh file, into text files (pre-files). It packs integer type information with a Stream Binary format in pre-files that are portable between machines. The files are generated to ensure fast read performance on different file-systems, such as Lustre and General Parallel File System (GPFS). A new subroutine has been added to the DSEM code to read the startup files using parallel MPI I/O, for Lustre, in a way that each MPI rank acquires its information from the file in parallel. In case of GPFS, in each computational node, a single MPI rank reads data from the file, which is specifically generated for the computational node, and send them to other ranks on the node using point to point non-blocking MPI communication. This way, communication takes place locally on each node and signals do not cross the switches of the cluster. The read subroutine has been tested on Argonne National Laboratory's Mira (GPFS), National Center for Supercomputing Application's Blue Waters (Lustre), San Diego Supercomputer Center's Comet (Lustre), and UIC's Extreme (Lustre). The tests showed that one file per node is suited for GPFS and parallel MPI I/O is the best choice for Lustre file system. The DSEM code relies on heavily optimized linear algebra operation such as matrix-matrix and matrix-vector products for calculation of the solution in every time-step. For this, the code can either make use of its matrix math library, BLAS, Intel MKL, or ATLAS. This fact and the discontinuous nature of the method makes the DSEM code run efficiently in parallel. The results of weak scaling tests performed on Blue Waters showed a scalable and efficient performance of the code in parallel computing.

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