DNS of Turbulent Flow on an IBM p690 Cluster

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Introduction

This abstract describes work in progress on two DNS codes, one designed for incompressible flows in simple geometries, using a pseudospectral method, and the other for compressible flows, using finite differences. The spectral code is that described by Sandham and Howard in [1], and used for the simulation of plane channel flow; the finite difference code has previously been used to study compressible channel flow [5], and shock/boundary-layer interaction [6].

DNS of Incompressible Channel Flow

Turbulent Plane Poiseuille flow is studied using a spectral discretization (Fourier in the two periodic directions tangential to the walls, and Chebyshev tau in the wall normal direction). Discretization in time is by compact third order Runge-Kutta for convection and Crank-Nicolson for the diffusion and pressure terms. The numerical method applies an influence matrix technique (so as to allow the implicit treatment of diffusion); it is described briefly in [1], and in more detail in [3] and [4].

The evaluation of the nonlinear terms is carried out pseudospectrally; this requires a transform to real space and back again at every Runge-Kutta step. This is done by transforming the data in 2-D planes, performing a global transpose, and then transforming the data in the third direction. Dealiasing is performed at the same time using the '3/2 rule'.

The present simulation is carried out at a Reynolds number of 1440 (based on friction velocity and channel half-width), which is the highest attempted to date for a flow of this kind; it is the latest in a series beginning with Re = 90, and including simulations of the same flow at Re = 180, Re = 360 and Re = 720. It is hoped that it will provide a significant amount of new data pertinent to turbulence modelling and LES research.

This range of available results means that while the state of the art in DNS remains severely restricted by Reynolds number, it is now possible to study trends with respect to Reynolds number variation for some simple flows like this one. In order to facilitate this, statistical results obtained using the DNS are published on the WWW [2].

DNS of Compressible Turbulence

A code for the simulation of compressible turbulence has been developed at Southampton, based on a stable high-order numerical scheme. This is made possible by an 'entropy splitting' technique, whereby the inviscid flux derivatives are split into a conservative and a non-conservative part [8]. Splitting of the flux function itself is not required, with the benefit that the method can still be expressed in terms of the usual conservative variables [5].

The result may be viewed as a form of conditioning, with a number of desirable properties. It has been found that, for smoothly varying flows, minimal additional numerical dissipation is required when using entropy splitting in conjunction with non-dissipative central difference schemes [7], while the non-conservative part of the flux derivative appears not to

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interfere with the correct prediction of shock locations [5]. The use of high-order non-dissipative schemes is to be desired for turbulence simulations, as the alternative of grid refinement is costly - three spatial dimensions are involved, and, since the time discretization is usually at least partly explicit, there are undesirable consequences for the size of the permitted time step as well.

In order to be useful in most physically relevant calculations, stable high order interior schemes need to be accompanied by compatible boundary treatments. Stability can be achieved by reducing the order of accuracy at the boundary; it is, however, possible to retain the accuracy of the interior scheme by constructing discrete operators that satisfy a summation-by-parts (SBP) rule. Such a scheme has been implemented in the code.

Some Experiences with Contemporary Parallel Architectures

The intention is to employ these codes on an IBM p690 cluster recently installed at Daresbury Laboratory. This machine is composed of 40 compute nodes, each containing 32 processors and connected via an IBM *Colony* switch.

The theoretical peak performance of each processor is 5:2 GFlops, so that of the whole machine is 6:66 TFlops, of which about 3:2 can be realized in practice on LINPACK (specifically, the R_{max} figure). By this measure, the machine is ranked 9th in the world.

Both codes have also been tested on the 768 processor Cray T3E and the 512 processor Origin 3800 provided by CSAR at Manchester.

DNS of Incompressible Channel Flow

This simulation requires a 1024x1024x480 grid at Re = 1440. The memory requirements are such that the T3E cannot be used. The IBM and SGI machines have sufficient memory; however, it is found that the speed of accessing it (both locally and by message passing) limits performance.

The global transpose for the evaluation of the nonlinear terms comprises almost all the communication requirements of the simulation, and it is this step that limits the scalability of the code.

Various methods of performing this transpose were investigated, using combinations of blocking, buffered, asynchronous, and one-sided MPI communication, as well as MPI collective operations. Optimum performance was obtained by amalgamating as much communication as possible, and by ordering it appropriately. This was found to be particularly important on the IBM machine. Overlapping communication with computation was not found to result in any performance benefit on either IBM or SGI.

DNS of Compressible Turbulence

The parallelization of the code (carried out by M. Ashworth at Daresbury Laboratory), exploits the IBM Regatta architecture very effectively. 6-7 times speedup is observed over the Cray T3E, with approximately linear scaling on both platforms.

Future work planned with this code will involve more complex geometries than have previously been investigated, including cavity flows and the near field of a turbulent jet (including thick trailing edges). In order to simulate these cases efficiently, a capability for multiple-block grids has been added, implemented using nested MPI communicators.

Parallel IO has also been added.

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