Recent Trends in HPC at HPCL, IIT Kanpur

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Abstract

An account of work done in High Performance Computing Laboratory (HPCL), I. I. T. Kanpur, in developing high accuracy methods for DNS and LES is provided here [1]. All the simulations are done on HCL clusters with REDHAT LINUX distribution with support for distributed programming (MPI) and shared memory platform (OpenMP). They all relate to scientific computing and broadly categorized as:

1. High Resolution/Accuracy Schemes

DNS methodologies are developed for problems related to flow instability, transition and turbulence [1]. For problems of turbulence, a wideband of spatial (wavenumbers) and temporal scales (frequencies) are excited which require huge computational resources if traditional methods are employed. Although Large Eddy Simulation is an alternative to solve problems of turbulence, ideally one would like to achieve solutions of Navier-Stokes equations without simplifying assumptions or modeling. In expanding scope of HPC, one requires better methods based on sound analysis [2,4] and by optimizing schemes not only to achieve higher resolution, but also to support physical properties [3,4]. The initiative on developing numerical schemes for the accurate evaluation of convective terms result in saving grid points in each direction by a factor of five to ten [5,7]. One class of such schemes, namely the Optimal Upwind Compact Schemes, allow reduction of errors related to dispersion and phase. The calculations are all performed in the transformed plane and problems of two- and three-dimensional geometries have been solved/tackled.

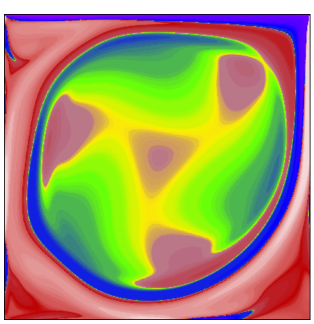

Figure 1: Vortical structures inside a square lid-driven cavity for Re=10,000.

We have also investigated on optimized methods those provide excellent dissipation discretization [5,6], that also helps control aliasing error for high Reynolds number problems. A typical high accuracy solution for high Reynolds number square lid driven-cavity flow is shown in Fig. 1. The solution identifies triangular vortex computationally at the core - that has only been shown experimentally before. These near-spectral accuracy methodologies have been extended for parallel computing of multi-dimensional flows [7].

2. Flow Past a Circular Cylinder Executing Rotary Oscillations

This problem of receptivity to wall oscillation in azimuthal direction, displays flow instabilities by the mechanism of *bypass transition* that leads to large drag reduction. This event creates large bandwith of wavenumbers and frequencies and poses a significant challenge in computing this flow. In Fig. 2, typical results are shown for this flow.

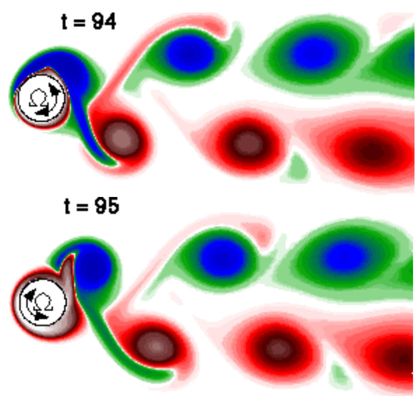

Figure 2: Flow past a circular cylinder executing rotary oscillation for Re=150.

3. Hypersonic Receptivity

In solving this problem, we have used the parallel compact schemes developed in [7], by Schwarz domain decomposition technique. The receptivity of hypersonic boundary layer to freestream vortical excitations [8] has been studied by solving unsteady, 3D, compressible Navier-Stokes equations for

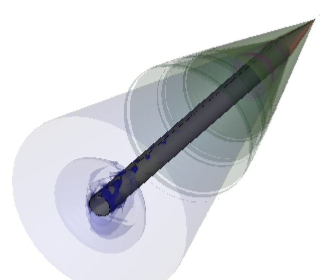

Figure 3: Pressure contour surfaces for hypersonic transition over a tangent-ogive body at Mach no. 4, Re=1.12×10^6.

a tangent-ogive body configuration on a cluster of 20 processors using [7]. The shock-vortex interactions are accurately captured and the linear and nonlinear instabilities can be identified in Fig. 3.

4. Chimera/Overset Grid Methods

One of the limitations of compact schemes is their inability to solve problems with complex geometries, as the method works on structured grid. To alleviate this, Chimera/Overset grid method has been used by us where the problem is solved in overlapping structured grids. The robustness of this methodology is demonstrated in an exercise for flow past two side-by-side cylinders and the results are shown in Fig. 4 [9]. This method can be adopted for store separation dynamics of rockets and projectiles, multi-element airfoils calculations etc.

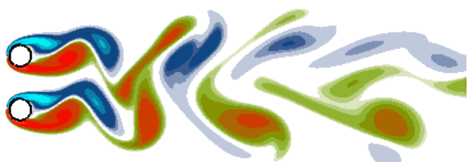

Figure 4: Flow past two circular cylinders placed normal to the oncoming flow using the Chimera method for Re=100.

5. Accelerating Computations

While we have made substantial progress in discretizing spatial derivatives, in recent times we have performed dispersion error analysis and proposed time-advancement schemes of Runge-Kutta type [10] that optimizes error and accelerate computations by factor of two for two-dimensional flow problems. Figure 2, was obtained by using this optimized time advancement scheme, where one lesser stage of computation is performed along with the increase of time step by a factor of 1.5 times- overall providing the above acceleration. We have been able to speed up all our computations by adopting this method and a typical solution is shown in Fig. 5, which used this optimized time advancing scheme, along with filter discussed next.

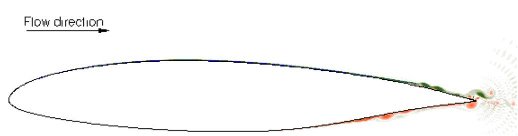

Figure 5: Vortical structures for SHM-1 airfoil for Re=10.3×10^6.

6. Filters & LES

Over the last few decades, LES has become an important tool in predicting large scale features in high Reynolds number flows. DNS is impractical here as one would require 'astronomical' (in a figurative sense) grid points to reveal the finest features present in these flows. The CFD community in performing classical LES is constrained by (i) filtering the governing equation; (ii) using additional subgrid scale models and (iii) special treatment of flows near the boundary. Explicit filters have been traditionally used for numerical stability. But, they are now being explored as LES tools applied on the solution of governing equations, without facing any of the above problems of traditional LES. We have analyzed various schemes and developed methodologies based on physical principles, for simulation of turbulent flows [11]. This has been successfully used in simulating bypass transition at high Reynolds number flow for Natural Laminar Flow, SHM-1 airfoil. An important issue of filtering multi-dimensional problems is retaining isotropy of the solution. We have developed novel isotropic filters that preserve isotropy of the solution with significant reduction in computations. In Fig. 6, the effects of isotropic filter is compared with the solution obtained without the filter for the problem in section 2. The solution without the filter blows up subsequently.

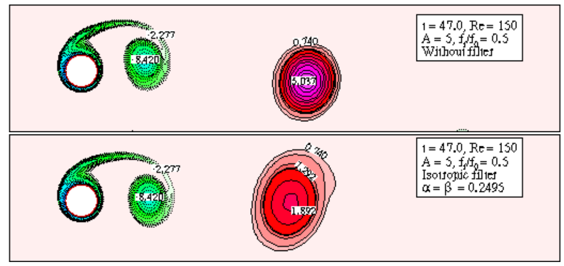

Figure 6: Illustration of the effect of isotropic filters.

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