Direct Numerical Simulation of Turbulent Natural Convection Flows Using PC Clusters

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Summary

PC clusters with conventional 100 Mbits/s networks provide a high computing power-cost ratio compared with conventional parallel computers. However, their low bandwith and high latency are serious obstacles that prevent their efficient use for many conventional parallel CFD algorithms.

A code for the direct numerical simulation of turbulent flows, that provides fairly good scalability up to about 36 processors has been developed. It is based on a finite control-volume formulation, and uses a spectro-consistent numerical scheme. The main bottleneck, the Poisson equation, is solved with a Direct Schur-Fourier Decomposition. This algorithm only needs one all-to-all communication episode to solve the Poisson equation almost to machine-accuracy and therefore is specially useful on high-latency computers.

The statistics of a turbulent natural convection flow in a tall cavity will be presented and compared with the previous results available from the literature, that assume a two-dimensional behaviour.

Introduction

The so-called *Beowulf clusters* (www.beowulf.org) of PCs running Linux have consolidated as a very cost-effective tools for high performance computing. However, specially if low cost 100 Mbit/s networks are used, their comunication performance is poor compared with their computation performance. This is a serious obstacle for the efficiency of the parallel algorithms on PC clusters. Parallel algorithms tolerant to loosely coupled computers must be developed in order to use efficiently their CPU potential.

Direct numerical simulation (DNS) of transition and turbulence flows is one of the typical examples of an application with huge computing power demands, that needs parallel computers to be feasible. Despite the interest of DNS for engineering applications, its cost is still too high to be used for design purposes. With the increase in computing power provided by the low cost PC clusters, this situation can change, specially for the case of low-Reynolds number and transition flows, that are relatively more accessible for DNS and more difficult to predict with RANS and LES turbulence models.

A parallel code for the direct numerical simulation of turbulent incompressible flows has been developed. To solve the Poisson equation, an algorithm called Direct Schur Fourier Decomposition (DSFD), specially designed for loosely coupled parallel computers is used [1]. This allows the code to scale up to 36 processors in a low cost PC cluster.

The aspects to be covered in the presentation are: a short description of the DSFD algorithm for Poisson equation, the spectro-consistent spatial discretization, the method used to verify the code and the DNS results in a natural convection turbulent flow.

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Numerical methods and parallel algorithms used

Spatial decomposition is the typical approach used to parallelize CFD codes. For DNS codes, the momentum and energy equations are usually discretized with a fully explicit method and their parallelization is straightforward. Even if an implicit method is used, as the time steps are small, the equation systems can be efficiently solved with a parallel iterative method. The main problem is the Poisson equation arising from the mass conservation equation. It has to be solved almost to machine accuracy for each time step or iteration and couples distant points of the domain. If loosely coupled parallel computers are used, the problem becomes even harder. In our code, Direct Schur-Fourier Decomposition method [1] is used to solve the discrete Poisson equation. DSFD is based on a combination of a direct-Schur [2] method and a Fourier decomposition.

The well known Fourier decomposition methods [3], under certain conditions, allow to transform a three-dimensional equation system into a sequence of two-dimensional systems, that can be solved simultaneously using any direct or iterative method. On tightly coupled parallel computers, Fourier decomposition provides a method for the paralalelization of Poisson solvers. However, this approach is not efficient for loosely-coupled parallel computers, because it requires the paralelization of the FFT of a large number of relatively short vectors, each of them distributed among all the processors. This operation, to the knowledge of the authors, can not be done efficiently on a loosely-coupled computer.

Instead, DSFD uses a domain decomposition in the two directions orthogonal to the Fourier decomposition. The pentadiagonal equation systems are solved with a parallel direct Schur decomposition, that is based on the fact that the matrix of coefficients of each pentadiagonal equation remains constant during all the fluid flow simulation. This allows us to evaluate and store the inverse of the interface matrix of each pentadiagonal equation in a pre-procesing stage. Then, in the solution stage, all the pentadiagonal systems are solved together. Only one all-to-all comunication episode is needed to solve each three-dimensional Poisson equation to machine accuracy.

More details of the algorithm will be given in the presentation, including an enhanced parallel method to calculate the inverse of the interface matrix, the treatment given to the singularity of the three-dimensional Poisson equation, and the stability of super-critical two-dimensional flows associated with DSFD. Computing times and speed-ups obtained for meshes up to 3.1×10^6 nodes and 36 processors in a Beowulf cluster will be presented.

The spatial discretization is carried out with a spectro-consistent second-order scheme [5,6] that allows an exact verification of the global kinetic-energy balance even on coarse meshes. Work is in progress to extend the method to fourth order schemes. However, this will increase the complexity of the discrete Poisson equation and modifications in the DSFD algorithm will be necessary.

The time discretization is based on a fully explicit second-order Adams-Bashforth scheme for body forces, diffusion and convection terms, and an implicit first-order Euler scheme for pressure-gradient term and mass-conservation equation. Only one iteration per time step is needed to solve almost to machine accuracy the pressure-velocity coupling.

The Method of Manufactured Solutions (MMS) [7], based on the systematic discretization convergence tests using analytic functions, has been used for the verification of the code. In order to obtain a qualitative estimation of the accuracy of the DNS solutions, statistic results with different meshes have been obtained and compared.

Turbulent Thermal Driven Cavity

The first direct numerical simulations carried out with the present code are of natural convection flows in differentially heated cavities (DHC). In a general DHC problem, two opposite vertical walls of the cavity, $y=0$ and $y=L_y$ are kept isothermal at temperatures T_c and $T_h > T_c$. The horizontal walls $z=0$ and $z=L_z$ can either be adiabatic ($\frac{\partial T}{\partial x}=0$) or perfecly conducting (i.e.,with a linear temperature profile between the hot and the cold temperatures). If Boussinesq approximation is used, DHC problem is governed by $Ra_z = \frac{\beta \Delta T L_z^3 g}{\alpha \nu}$ and $\Pr = \frac{\nu}{\alpha}$ numbers and the geometric aspect ratios $A_z = \frac{L_z}{L_y}$ (height aspect ratio) and $A_z = \frac{L_x}{L_y}$ (depth aspect ratio). For three-dimensional configurations, the vertical planes that close the cavity in the direction orthogonal to the main flow, x=0 and x=L_x can be adiabatic solid walls $\boldsymbol{u}$=0, $\frac{\partial T}{\partial x} = 0$) or a periodic behaviour can be assumed, $\varphi(x,y,z)=\varphi(x+L,y,z)$. Non-slip $\boldsymbol{u}$=0) boundary condition is always used for the other four planes.

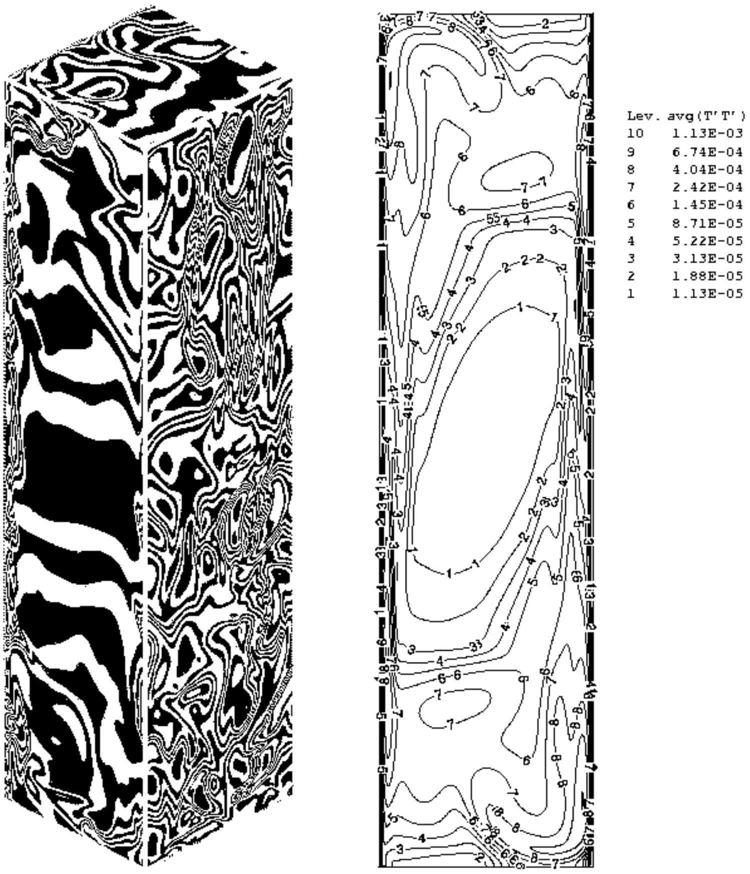

Fig. 1. Illustrative results. Left: Instantaneous temperature distribution. Right: Map of $\overline{T'T'}$.

In our case, a situation with A_z=4, A_x=1, Pr=0.71, Ra_z=6.4x10^8 and periodic boundary conditions has been selected. It is an extension to three-dimensions of one of the two-dimensional problems studied in detail in [8]. This configuration is of interest because the majority of the previous works concerning direct numerical simulations of turbulent natural convection flows assumed the flow to be two-dimensional. The effect of the three-dimensional fluctuations over the averaged flow is not precisely known yet. Statistics ($\overline{u}$, $\overline{T}, \overline{Nu}$, $\overline{u_i' u_j'}$, $\overline{u_i' T'}$, $\overline{T'T'}$) of the two-dimensional and three-dimensional flows will be presented.

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