Direct numerical simulation of lid-driven cavity flow within a 3D inhomogeneous domain on an NEC-SX4 supercomputer

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Abstract

A tractable global Chebyshev spectral method has been implemented for the solution of the incompressible Navier-Stokes equations in three-dimensional rectangular domains where the flow is inhomogeneous in all spatial directions. The solution procedure for a problem requiring high resolution reaches an average processing rate of 1.9 Gigaflops on a single processor of the NEC-SX4. A parallel version of the algorithm on 16 processors runs at a sustained 26 Gigaflops. A direct numerical simulation with high resolution is performed within a cubical lid-driven cavity at high Reynolds number. The dominant features of the mean flow are reported.

1 Introduction

The direct numerical simulation (DNS) approach consists of accurately solving the full nonlinear, time-dependent Navier-Stokes equa-
tions without any empirical closure assumptions for prescribed initial and boundary conditions. A complete description of the flow field (velocity and pressure) as a function of space and time is provided by DNS.

Due to their very high asymptotic accuracy, spectral methods are the preferred method for doing DNS. But their use is limited to simple geometries that can produce efficient algorithms. Until recently, spectral DNS methods have been restricted to flows that have at least one periodic direction, owing to the great efficiency of the use of Fourier expansions.

It has now become possible to use spectral methods for doing DNS in domains that are inhomogeneous in all three spatial directions. This has been achieved by developments in advanced algorithms and parallel machines with fast vector processors. The following sections discuss the key issues that make it possible to perform an efficient direct numerical simulation of high resolution within a cubical lid-driven cavity at high Reynolds numbers.

2 Governing equations

The present method is applied to the flow domain shown in figure 1. The fluid is enclosed by six solid, smooth walls of which only the top is set in horizontal motion and drives the flow within the cavity. The equations governing the fluid flow inside the domain, $\Omega$, are assumed to be the incompressible Navier-Stokes system, which may be written as

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla p + \nu \nabla^2 \mathbf{u} \quad ,$$

with the incompressibility constraint,

$$\nabla \cdot \mathbf{u} = 0 \quad ,$$

where $\mathbf{u}$ is the velocity vector, $\nu$ the kinematic viscosity and $p$ the pressure (divided by the density). On the boundary $\partial \Omega$, the velocity is specified to be zero everywhere except at the lid, $y = h$, where it is prescribed (see below).

3 Numerical method

The velocity and pressure fields are expanded in tensor product of Chebyshev polynomials in three dimensions. The Chebyshev collo-
cation method consists of enforcing the differential equations at the Chebyshev-Gauss-Lobatto collocation points exactly [2]. The system of equations is treated in the physical space on these collocation points for each variable with associated boundary conditions.

![Diagram of three-dimensional lid-driven cavity flow](image)

Figure 1: Geometry and boundary conditions on the top-wall of the three-dimensional lid-driven cavity flow.

The non-linear terms are taken as a source term, evaluated explicitly in time by extrapolation (see below) based on the skew-symmetric form

\[ N(u) = \frac{1}{2}[(u \cdot \nabla)u + \nabla(u \cdot u)]. \]

Then, the key to the method’s efficiency relies on the splitting of the Stokes equations in such a way that the cost of enforcing the continuity is drastically reduced. The time advancement is based on a two-stage procedure, to enforce the incompressibility constraint, and then to incorporate the viscous diffusion. This method, named projection-diffusion (PRDI), was proposed by Batoul & al. [1] and analysed by Leriche and Labrosse [10]. It appears similar to a fractional step or high-order splitting methods [4] since it proceeds with similar steps. However, the decoupling is now defined independently of any temporal scheme avoiding any time splitting errors. A brief description of its present implementation is given below. An inter-
mediate acceleration vector \( a \) is defined as the difference
\[
a = \frac{\partial u}{\partial t} - \nu \nabla^2 u.
\]

The first step in the solution procedure is given by
\[
a + \nabla p = \mathbf{N}(u) \quad \text{in } \Omega'
\]
\[
\nabla \cdot a = 0 \quad \text{in } \overline{\Omega}
\]
\[
a \cdot \mathbf{n} = \left( \frac{\partial u}{\partial t} - \nu \nabla^2 u \right) \cdot \mathbf{n} \quad \text{on } \partial \Omega,
\]
where \( \mathbf{n} \) is the vector normal to \( \partial \Omega \). We denote the closure of \( \Omega \) by \( \overline{\Omega} \) and \( \Omega' \) stands for
\[
\Omega_1 = [-h, +h] \times [-h, +h] \times [-h, +h]
\]
\[
\Omega_2 = [-h, +h] \times [-h, +h] \times [-h, +h]
\]
\[
\Omega_3 = [-h, +h] \times [-h, +h] \times [-h, +h]
\]
where \( \Omega_i \) is the domain in which the \( i \)-th component of equation (3) is solved. The second step is the solution of the system
\[
\frac{\partial u}{\partial t} - \nu \nabla^2 u = a \quad \text{in } \Omega
\]
\[
u u = f \quad \text{on } \partial \Omega.
\]
Using the continuity constraint and the boundary condition for the velocity, equation (5) is replaced by
\[
a \cdot \mathbf{n} = \left( \frac{\partial f}{\partial t} + \nu \nabla \times (\nabla \times u) \right) \cdot \mathbf{n}
\]
It has been shown [10] that this form preserves the ellipticity of the discrete Stokes operator. In practice, this equation is used to estimate the boundary values of \( a \) at discrete time intervals by extrapolating the terms on its right-hand-side with a scheme having temporal accuracy equivalent to that used for the time-integration of the viscous part of the problem – equation (15) below. This preserves the overall temporal accuracy of the integration procedure. The exact formula used is that proposed by Karniadakis & al. [4]. The same formula is also used to extrapolate the non-linear terms in time.

The system of (3), (4) and (11) is discretised using Chebyshev polynomial expansions for the velocity and pressure fields of the same order.
(this is known as $IP_N$, $IP_N$ type of approximation). The discrete set of equations is modified by incorporating the boundary conditions in the momentum equation. Therefore one may write the equation for the grid-point vectors $\tilde{a}$, $\tilde{p}$ and $\tilde{u}$

\[
\tilde{a} + G\tilde{p} = M(\tilde{u}) \tag{12}
\]

\[
D\tilde{a} = 0 \tag{13}
\]

where $G$ is the discrete gradient operator including the boundary conditions, $D$ the discrete divergence operator, and $M(\tilde{u})$ the corresponding discretized version of $N(\mathbf{u})$ operator. The values of $M(\mathbf{u})$ at a given time level are obtained by extrapolation from previous time levels [4]. By taking the divergence of the first equation and with the use of the incompressibility (13), one finds an equation for the pressure field given by

\[
DG\tilde{p} = DM(\tilde{u}) \tag{14}
\]

In spectral collocation method, the matrix on the left of this equation is full. Its inversion would normally involve substantial, if not prohibitive, costs in computer memory and execution times. However, the geometry of the computational domain allows the splitting of the pressure matrix into tensor products of smaller 1D matrices (order $N^2$ where $N$ is the number of polynomials along one direction) [3], which involves a pre-processing stage that reduces the operation count of the time stepping algorithm substantially. In addition, this process gives direct access to the spectrum of the pressure operator which can be easily filtered to remove the spurious pressure modes [10].

Following the estimation of the pressure field, the vector $\tilde{a}$ can be calculated from (12). This in turn enables the solution of the second step in the algorithm: equations (9) with the boundary conditions (10). A second order Euler scheme is used for advancing in time. The fully discrete form is

\[
\frac{3\tilde{u}^{n+1} - 4\tilde{u}^n + \tilde{u}^{n-1}}{2\Delta t} - \nu L\tilde{u}^{n+1} = \tilde{a} \tag{15}
\]

which is implicit in the viscous terms. $L$ is the discrete Laplacian and $\Delta t$ is the time step. This requires the solution of a vector Helmholtz problem for every step. As with the pressure operator, $L$ can also be
cast into the tensor product form with substantial gains in computational efficiency.

The stability of the Stokes splitted scheme has been analysed in [10]. The explicit evaluation of the rotational boundary term does not prevent the second order in time schemes from being unconditionally stable. The Navier-Stokes scheme is subject to restrictions in the size of the time step due to the explicit advancement of the non-linear terms.

4 Some comparative data with the Uzawa approach

To decouple the velocity and pressure fields by the Uzawa method is, to a certain extent, a reference approach for solving the Stokes problem accurately. Nonetheless, this method is very expensive when the diffusion terms are implicitly evaluated with time. The authors' point of view is that the PRDI decoupling is an interesting alternative to get equivalent results [6] at a significantly reduced cost. A few comparative numerical results are therefore given for the PRDI and the unique grid \((P_N, PN-I)\) Uzawa solvers in this section.

First, for the asymptotic operation count, a comparison is given in [10]. It indicates that the Uzawa method is \(7 N_{it}\) times more expensive than the PRDI solver, where \(N_{it}\) stands for the iteration number required for the preconditioned iterative Uzawa solution to converge to the machine accuracy. \(N_{it}\) is very sensitive to the physical configuration (the Reynolds number values for instance), to the number of collocation points and the time step size [8].

Finally, the PRDI and the preconditioned Uzawa Stokes solvers are compared in a benchmark Navier-Stokes application, the two-dimensional regularized lid-driven square cavity \([0, 1]^2\) at a Reynolds value of 1000, where the flow is steady. Both Navier-Stokes solvers have a second order accuracy in time. Owing to the absence of an analytical solution for this problem, the solutions based on \(129^2\) collocation points with the Uzawa and the PRDI solvers have been used as the references for calculating the errors. Both algorithms exhibit comparable error drops as the order of the polynomial expansion is increased [10].
5 DNS of the driven cavity flow

5.1 Physical and computational parameters

It is common practice for this type of simulation to set the lid velocity to a constant value even though it is well known that the discontinuity in the boundary values of the velocity cannot be physically correct [5]. The numerical results are usually assumed to be uninfluenced by such discontinuities in the data. This approach cannot be used with global spectral methods such as the one used here. The velocity profile for the lid is therefore specified as

\[ u(x, h, z) = U_o(1 - (x/h)^{18})(1 - (z/h)^{18})^2 \] (16)

which gives \( u(x, h, z) > 0.85U_o \) over 75% of the lid area. \( U_o \) is the maximum velocity occurring over the lid. The choice of the exponents was arrived at after considering the ability of the polynomial expansion to capture the sharp gradients near the edges of the lid [7]. Note that the exact boundary conditions in an experiment are unknown. The Reynolds number based on the maximum lid velocity is

\[ Re = U_o2h/\nu = 12000. \]

The number of polynomials used along each direction is 129 giving a total of 2.14 \( 10^6 \) collocation points in space. The size of the time step was 0.0025\( h/U_o \). The execution speed on a single processor of a NEC-SX4 was 8.8\( \mu s \) per collocation point per time step. The next section discusses the key features leading to an efficient vectorized and parallelized code.

5.2 Parallelization and performance of the code

As mentioned in Section 3, the geometrical simplicity of the computational domain allows the inversion of the pressure operator and the Helmholtz vector operator by the fast diagonalization method [3]. These inverse are made of tensor products of smaller matrices, one per spatial direction. Most CPU time is consumed by the inversions of these operators which consist of matrix-matrix multiplication. The generalized matrix-matrix multiplication is based on the Fortran NEC-SX internal routines, optimally vectorized for a single processor. These routines can also be used in a very simple way within a parallel program to deliver the optimum parallel performance for
the different matrix operations presented above. On 2 processors, the computation of \( C = A \times B \) is divided into the following 2 calculations \( C_1 = A \times B_1 \) and \( C_2 = A \times B_2 \), where \( C = [C_1, C_2] \) and \( B = [B_1, B_2] \). In most cases, due to the tensor product nature of the operator, the matrices \( B \) and \( C \) are of the size \( N \times N^2 \). The matrix \( A \) is of size \( N \times N \). This means that the partial matrix multiplication \( C_i = A \times B_i \) could be done very efficiently on one vector processor. Table 1 gives the parallel performance of the code with the final mesh \( 129^3 \) as a function of the number of processors on a NEC-SX4: the speedup factors, the GFLOPS sustained and the CPU time in seconds per time step. The degree of parallelism is 99%. The execution speed on 16 processors on a NEC-SX4 is 0.7 \( \mu \)s per collocation point per time step. The parallel Chebyshev code exhibits a perfect linear scale with a number of up to 8 processors, whereas the performance of the code slows down, probably due to the too small size of submatrices on each processor.

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</table>

Table 1: Speedup characteristics of the driven cavity DNS simulation as a function of the number of processors on a NEC-SX4 (mesh \( 129^3 \)).

5.3 Some DNS results

The initial conditions of the simulation consisted in setting the lid in motion at \( t = 0 \) while the fluid inside the cavity was at rest. The initial Reynolds number \( Re \) was of the order of 1000. It was increased progressively until the final value was reached. With the final Reynolds number, the simulation was run for \( 1900h/U_o \) units in time of which the last \( 1000h/U_o \) were used for statistical analysis.

The statistically steady state of the simulation was judged from the evolution of the volume averaged kinetic energy, dissipation rate and wall-averaged stress over the lid. During the last part of the simulation their maximum variations from their respective mean values were of the order of a few percent. This sample is quite sufficient for zero, first and second order statistics whereas some asymmetry about the mid-plane in the higher order statistics has persisted.
Prasad and Koseff [11] have measured some of the velocity statistics within a cubical cavity at $Re = 10000$ (among others). The agreement between experiment and simulation data is very good for the mean velocity, but some differences are found between the two sets of $rms$ values, mainly due to measurement errors as the moving wall is approached. However, the details of the evolution of the flow-field of the simulation indicated that the statistics of the experiment may not have sufficiently converged [7].

The dominant feature of the mean flow is the large-scale recirculation which spans the cavity (figure 2). Away from the side walls, the mean transfer of momentum from the moving lid to the underlying fluid is dominated by viscous diffusion in a very thin region. The momentum diffusion from the top wall is self-convected towards the downstream edge of the cavity. This is dominated by the $u$ mean field, the fluctuating field being negligible in this area. Near the downstream wall the flow structure is dominated by its $v$ component. The structure of the downflow is similar to a plane wall jet which separates from the downstream wall. Two higher speed regions on each side of the symmetry plane concentrate into two distinct jets, impinging on the bottom wall at well defined points. At the impact location each downflowing jet is split into two opposite flow streams parallel to the bottom wall running approximately in the $x$-direction. On either side of the impingement point, the part of the flow heading towards the downstream wall rolls up into the corner spiralling vortex. A part of the fluid is also redirected towards the symmetry plane and another toward the side wall. Near the bottom wall, the flow field exhibits a turbulent behaviour. These turbulent structures are carried by the large scale recirculation towards the upstream wall. Two jets impinge on the upstream wall. Near the upstream vertical wall, on either side of the symmetry plane there is a region with higher vertical velocity. This has effects on the near-lid flow. About the symmetry plane dividing the cavity, there is a relative thin fast-flowing region with two wider but slower-flowing ones on each side. The instantaneous flow-field near the lid and downstream wall resembles the structure of the mean flow. The whole pattern is, of course, unsteady with pronounced displacements about the symmetry plane.

A more complete description of the mean velocity field and of the higher order statistics may be found in [7, 9].
6 Summary

The numerical solution of the incompressible Navier-Stokes equation in a rectangular domain using global Chebyshev expansions for the primitive flow variables has been implemented. The solution procedure enforces the incompressibility constraint ahead of the calculation of the viscous effects. This leads to a more tractable problem for the numerical evaluation of the pressure field. The direct simulation of the flow in cubical lid-driven cavity at a Reynolds number of 12000 using $129^3$ collocation points has been achieved.

Figure 2: Schematic showing the main features in a lid-driven cavity flow.

References


