

Multi-domain Fourier Algorithms for Parallel Solution of the Navier-Stokes Equations *

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Abstract

We present a parallel multi-domain algorithm for the solution of the incompressible Navier-Stokes equations. A high-order scheme is employed for the time discretization. The discretization in space is based on Fourier methods. For the interior subdomains we use an overlapping Local Fourier Basis technique, for the boundary subdomains - a non-overlapping Fourier-Gegenbauer method.

The matching of the local solutions is performed via a direct point-wise procedure on the interfaces, using properly weighted interface Green's functions. The unknown coefficients are found explicitly in terms of the jumps of the solution and its first derivatives at the interfaces.

The localization properties of the interface Green's functions are exploited in order to simplify the matching relations so that communication is reduced mostly to local data exchanges between neighboring subdomains. In effect, the parallel algorithm becomes highly scalable with the percentage of the global communications decreasing as the resolution requirements of the problem increase.

1 Introduction

Parallel multiprocessor computers are becoming indispensable for large-scale scientific computing, in particular, in computational fluid dynamics (CFD) where direct numerical simulations at high Reynolds numbers are one of the principle means of research.

The high performance of parallel machines can be realized only if effective parallel algorithms are supplied. An efficient parallel strategy for CFD problems is domain decomposition. The geometric domain decomposition (DD) is intrinsically suited for the purposes of parallelization since neighboring pieces of space (subdomains) can be allocated to processors with short communication

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links. Such a decomposition is in agreement with the natural data dependencies of elliptic and time-parabolic problems. The original problem is solved independently in each processor, then some patching procedure is employed to enforce the continuity conditions on the interfaces. Such a patching step requires communication between processors. The objective of any DD method is to minimize the interprocessor communication and the amount of data to be transferred in order to avoid communication and synchronization bottlenecks.

Numerical simulation of fluid flows at high Re numbers requires high resolution in time and space. Spectral methods, using series expansions in terms of polynomial or trigonometric functions, are most appropriate for such problems. For smooth flow fields these methods converge exponentially fast as the number of modes increases. However, all spectral methods are inherently global as they couple all variables in the domain for the computation of any local quantity. The implication of this fact for parallel processing is that parallel algorithms using spectral methods are expected to become inefficient in the case of massively parallel processor due to communication bottlenecks (but see [2] for the spectral element approach).

In [5, 6, 9] a low communication multi-domain approach is developed. A notable feature of this approach is that it makes use of Fourier methods for space discretization. A modified Local Fourier Basis (LFB) technique [1] is employed for the smooth decomposition of the original problem into subproblems. The use of the Fourier basis leads to a great reduction of the parallel complexity as it makes it possible to match independently each separate harmonic in the spectral space. Another important feature of this approach is that it takes advantage of the local behavior of the Green's functions employed to impose continuity conditions at the interfaces. As a result, the influence of remote domains on the processing at a particular location becomes negligible and the interprocessor communication is confined to local data exchange between neighboring units.

This paper is a further development of the local Fourier methods for the solution of PDEs in multi-domain regions. A novel feature of the present algorithm is the combination of the LFB technique, applied in the interior subdomains, and the Fourier-Gegenbauer (FG) method of [3] in the boundary subdomains. The use of a non-overlapping FG method enables us to treat non-periodic problems. The method is applied here to the incompressible Navier-Stokes equation for regions decomposed into parallel strips or rectangular boxes.

2 Formulation of the Problem and Numerical Schemes

We are interested in the numerical solution of the unsteady incompressible Navier-Stokes equations that govern viscous flows with constant properties:

$$\frac{\partial \mathbf{v}}{\partial t} = Re^{-1} \nabla^2 \mathbf{v} + \mathbf{N}(\mathbf{v}) - \nabla \Pi \quad \text{in } \Omega \subset R^2. \quad (2.1)$$

Here $\mathbf{v}(\mathbf{x}, t) = (u, v, w)$ is the velocity, subject to the incompressibility constraint

$$\nabla \cdot \mathbf{v} = 0 \quad \text{in } \Omega, \quad (2.2)$$

Π is the total pressure, and Re is the Reynolds number. The nonlinear term is written in the rotational form

$$\mathbf{N}(\mathbf{v}) = \mathbf{v} \times (\nabla \times \mathbf{v}). \tag{2.3}$$

The numerical solution of the problem (2.1)-(2.3) with specified boundary conditions requires discretization in both time and space.

2.1 Discretization in Time

The discretization in time is performed via the third-order splitting algorithm of [7]:

$$\frac{\hat{\mathbf{v}} - \sum_{q=0}^2 \alpha_q \mathbf{v}^{n-q}}{\Delta t} = \sum_{q=0}^2 \beta_q \mathbf{N}(\mathbf{v}^{n-q}), \tag{2.4}$$

$$\frac{\hat{\mathbf{v}} - \hat{\mathbf{v}}}{\Delta t} = -\nabla \Pi^{n+1}, \quad \nabla^2 \Pi^{n+1} = \frac{1}{\Delta t} \nabla \cdot \hat{\mathbf{v}}, \tag{2.5}$$

$$\frac{\gamma_0 \mathbf{v}^{n+1} - \hat{\mathbf{v}}}{\Delta t} = Re^{-1} \nabla^2 \mathbf{v}^{n+1}. \tag{2.6}$$

It consists of an explicit advection step (2.4), a global pressure adjustment for incompressibility (2.5) and an implicit viscous step (2.6).

The high-order approximation used for the pressure boundary conditions is:

$$\frac{\partial \Pi^{n+1}}{\partial \nu} = \nu \cdot \left[\sum_{q=0}^2 \beta_q \mathbf{N}(\mathbf{v}^{n-q}) + Re^{-1} \sum_{q=0}^2 \beta_q (-\nabla \times (\nabla \times \mathbf{v})^{n-q}) \right] \quad \text{on } \partial\Omega \tag{2.7}$$

where ν is the direction normal to the boundary.

Semi-implicit schemes of this type have much less severe restriction on the time step than fully explicit schemes. However the parallelization of such schemes is considerably more difficult because the boundary values at interfaces are not known explicitly and thus the local problems in subdomains are globally coupled.

2.2 Discretization in Space

The splitting procedure in time results in two types of elliptic equations, of the Helmholtz type

$$\nabla^2 u - \lambda^2 u = f(x, y), \tag{2.8}$$

and of the Poisson type

$$\nabla^2 u = f(x, y), \tag{2.9}$$

which have to be solved repeatedly (for each time step). The parameter λ in (2.8) is related to the time-stepping increment, $\lambda \propto 1/\sqrt{\Delta t}$.

The solution of Eq. (2.8), (2.9) is based on spectral methods with a Fourier basis. The Fourier method is the most efficient for the evaluation of spatial derivatives since the differential operators are represented in the transform space

by diagonal matrices so that harmonics with different wave numbers remain uncoupled. Another advantage of the Fourier method, when compared to Chebyshev or Legendre based methods, is that it has uniform resolution and is thus most appropriate for turbulence computations.

However it is well known that exponential (spectral) convergence of the Fourier series takes place only if it approximates a continuous periodic function. For a continuous but nonperiodic function, which has a discontinuous periodic extension, the truncated Fourier series does not converge uniformly near the boundaries giving rise to spurious oscillations of order $O(1)$ (Gibbs phenomenon). Therefore, when the Fourier method is applied to the solution of nonperiodic problems, like the elemental problems in subdomains, the key question is how to remove the Gibbs phenomenon.

We use two approaches in order to preserve spectral accuracy: a modified Local Fourier Basis (LFB) method of [1], implemented in the interior subdomains, and the Fourier-Gegenbauer (FG) method of [3]. In the first approach a smooth decomposition of the source function $f(x, y)$ is performed by using a system of overlapping bell functions. Then the local Fourier method is applied within each subdomain (see [5, 6] for more details).

The second approach makes use of re-expansion of the (local) Fourier partial sums into rapidly convergent Gegenbauer series. This technique is implemented in the subdomains adjacent to the boundaries where overlapping of two contiguous subdomains is not possible in the case of non-periodicity (e.g. for Dirichlet or Neumann boundary conditions).

The rapid convergence of the Gegenbauer series is related to the fact that the Gegenbauer polynomials $G_l^\lambda(x)$ are the solutions of singular Sturm-Liouville problems (l is the order of the polynomial; λ is a parameter appearing in the weight function $(1 - x^2)^{\lambda-1/2}$). Unlike the Chebyshev or the Legendre polynomials, the Gegenbauer polynomials constitute a two-parameter family. It is proven in [3] that in some parametric region λ , $l \propto N$ (N is the number of the Fourier coefficients, representing an analytic and nonperiodic function) the Gegenbauer series converges exponentially. The application of the FG method for the solution of nonperiodic PDEs is described in [10].

The FG method is a good choice for our purpose because it operates inside the interval where the function is defined, so that it does not require overlapping of subdomains. Also, the FG method has uniform resolution like the LFB method, so that both Fourier techniques are easily combined.

However, the resolution properties of the FG method are much worse than those of the Fourier method or the LFB method. Therefore the FG method by itself is too expensive to implement in the whole domain. The combination of both the LFB and the FG techniques meets the requirement of high efficiency.

3 The DD Technique in 1-D

We describe our Multi-domain Local Fourier (MDLF) approach as applied to a modified Helmholtz equation in 1-D:

$$\frac{d^2 u}{dx^2} - \lambda^2 u = f(x), \quad x \in [0, L]. \quad (3.1)$$

The computational interval L is divided into P pieces (subdomains) of arbitrary size l_n , $n = 1, 2, \dots, P$.

The algorithm consists of two steps:

Construction of the elemental particular solutions. We decompose (3.1) into local subproblems for $u_p^{(n)}(x)$, $x \in [\bar{x}_{n-1}, \bar{x}_n]$ and solve them independently in each subdomain with *arbitrary* boundary conditions on the interfaces. The LFB technique is employed in the interior subdomains and the FG technique in the boundary subdomains.

Matching step. The interface conditions impose matching of adjacent local solutions at $x = \bar{x}_n$: $u_p^{(n)} = u_p^{(n+1)}$, $\frac{d}{dx}u_p^{(n)} = \frac{d}{dx}u_p^{(n+1)}$. The matching procedure makes use of the properly weighted interface Green's functions $h_{\pm}^{(n)}(x)$ which satisfy the homogeneous form of (3.1). For each interface \bar{x}_n , these are two exponential functions decaying away on each side.

The smooth global solution is a linear combination

$$u = \bigcup_{n=1}^P u^{(n)}, \quad u^{(n)} = u_p^{(n)} + A_n h_+^{(n)} + B_n h_-^{(n)} \quad (3.2)$$

The unknown coefficients A_n , B_n can be found explicitly in terms of the jumps of $u_p^{(n)}$, $du_p^{(n)}/dx$ at the interfaces $x = \bar{x}_n$ (see [6] for more details).

This two-step algorithm can be viewed as a reduction of the full matrix, representing the elliptic operator in (3.1), to a block-diagonal form (see [4]). It results in a great reduction of the parallel complexity. Instead of a global coupling of the collocation points in the whole domain (which necessitates a global data transfer), the interaction is confined mostly to the neighborhood of the subdomain of interest. However, all interface points remain coupled globally.

An important feature of the MDLF approach is that it takes advantage of the local behavior of the interface Green's functions in order to decouple the matching relations. For small enough time steps Δt the functions h_{\pm} decay rapidly away from the interfaces so that the influence of remote interfaces become negligible. In effect, only local communication between neighboring subdomains (processors) is important. Note that the localization property of the modified Helmholtz operator, resulting from an implicit time discretization procedure, reflects the locality of the diffusive linear operator in the evolution problem (2.1).

On the contrary, the Poisson equation (2.8) describes equilibrium processes with global interactions. Therefore the solution of this equation requires global communication between subdomains. Nevertheless, we will show that in two (or more) dimensions the necessary global communications constitute only a small percentage of the required communication.

4 Extension to 2-D

The previous MDLF technique can be extended to two dimensions without loosing the property of locality. We consider a computational region $\Omega = (0, L_x) \times (0, L_y)$ divided into parallel strips or rectangular cells.

Case of strips. After applying the FFT in the periodic direction y along the strips we get a set of *uncoupled* 1-D ODEs for the Fourier coefficients $\hat{u}_k(x)$:

$$\frac{d^2 \hat{u}_k^{(n)}}{dx^2} - \lambda_k^2 \hat{u}_k^{(n)} = \hat{f}_k^{(n)}(x) \quad (4.1)$$

where $\lambda_k^2 = \lambda^2 + k^2$ for the modified Helmholtz equation and $\lambda_k^2 = k^2$ for the Poisson equation. These problems are solved by using the 1-D routine, described in section 3.

An important observation is that even in the case $\lambda = 0$, $\lambda_k \neq 0$ for $k \neq 0$, the homogeneous solutions of (4.1) decay exponentially as functions of x . Thus, a global matching procedure is required only for the long waves, $k \leq k_*$, whereas the short waves, $k \geq k_*$, can be treated by using local matching on the interfaces. The cut-off wave number k_* should be chosen in accordance with the prescribed accuracy.

Let us denote the number of collocation points in the x and y directions as N_x and N_y , and define $N_y/N_x = P^\gamma$ where P is the number of subdomains. Then $\eta = 2k_*/N_y$ will be the relative amount of equations (modes) treated locally. It can be shown that for $\gamma = 0$, that is $N_x = N_y$, the relative amount of local communication $\eta \propto \sqrt{P}$. Another limiting case, $\gamma = 1$, corresponds to $N_x = \text{const}$, $N_y \propto P$ (the resolution is changed only in the direction of strips, e.g. the case of a long channel). In this case η is independent of P , i.e. the algorithm is fully scalable.

Case of cells. In this case the direct point-wise matching at all interface points (in 2-D), using the corresponding two-dimensional interface Green's functions, results in a large linear system. The use of the LFB technique allow us to perform matching in the Fourier space for each Fourier harmonic independently. The procedure consists of several matching steps alternately in x and y directions. The maximum precision is attained after 2 – 3 iterations (for more details see [9]). The analysis of scalability in this case is similar to the case of strips.

5 Results and Conclusion

To demonstrate the accuracy of the MDLF method we consider the Kovaznay flow [8], which is an exact solution of the Navier-Stokes system (2.1):

$$u = 1 - e^{\rho x} \cos(2\pi y),$$

$$v = \frac{\rho}{2\pi} e^{\rho x} \sin(2\pi y)$$

where $\rho = Re/2 - (Re^2/4 + 4\pi^2)^{1/2}$. The domain decomposition into strips is considered. The computational parameters are: $P = 4$, $N_x = 128$, $N_y =$

32, $Re = 40$. Fig.1 shows the error (in the maximum norm) as a function of Δt^3 . The linear dependence, which is in agreement with the third-order scheme (2.4)-(2.7), gives an evidence that the spatial errors are below the temporal ones in this range of Δt .

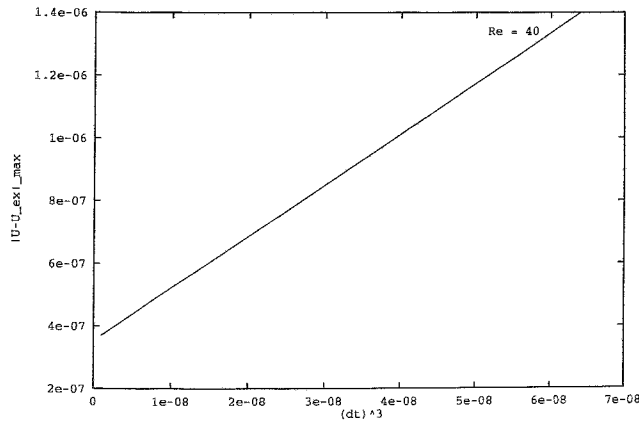


Figure 1:

To summarize, the MDLF approach, based on the local Fourier methods, overcomes most of the global coupling, inherent both in the use of a spectral method in space and an implicit discretization in time. It presents a low-communication, highly scalable parallel algorithm.

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