Contemporary Mathematics
Volume 157, 1994

Simulation of 3D Navier–Stokes Flows via Domain Decomposition by the Modified Discrete Vector Potential Model

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ABSTRACT. The Discrete Vector Potential (DVP) model integrates the primitive variable equations of internal flows of incompressible Navier–Stokes fluids. It provides exactly local and global mass conserving flow fields at each time step, [1]. This feature makes the DVP model expecially suitable for domain decomposition, as the "a priori" satisfaction of the mass conservation law in each subdomain avoids the numerical production of mass that is generally the main cause of the growth of spurious flow micro–structure at the interfaces.
In this work the application of a domain decomposition technique with a modified version of the DVP model is presented. The Modified Discrete Vector Potential (MDVP) model, adopted in each subdomain, allows to cut half of the total computational effort by solving the vector potential equations and still assuming boundary conditions in primitive variables. This results also in preserving the advantages of the original numerical model. The chosen solution technique consists of a multiplicative Schwarz procedure with overlapping subdomains.
Several numerical tests are described.

1. Introduction

The present work relates to the numerical study of the stability of the flow of the liquid phase of artificially grown crystals. Newtonian incompressible fluids in shallow open rectangular cavities with a horizontal differential of temperature are assumed as a mathematical model [2]. Our attention is focused on the determination of the unsteady solutions of the Navier–Stokes equations with buoyancy source term and Boussinesq approximation:

$$\begin{aligned} &\frac{1}{\sqrt{Gr}}\frac{\partial \mathbf{q}}{\partial t} + \nabla\cdot(\mathbf{qq}) = -\nabla p + \frac{1}{\sqrt{Gr}}\nabla^2\mathbf{q} - \frac{\mathbf{g}}{|\mathbf{g}|}T \\ &Pr\left(\frac{1}{\sqrt{Gr}}\frac{\partial T}{\partial t} + \nabla\cdot(\mathbf{q}T)\right) = \frac{1}{\sqrt{Gr}}\nabla^2 T \\ &\nabla\cdot\mathbf{q} = 0. \end{aligned} \tag{1}$$

1991 Mathematical Subject Classification. Primary 65M55, 65M06.
Supported by C.N.R. and A.S.I. (project n. 149 MSF).
This paper is in final form and no version of it will be submitted for publication elsewhere.

with appropriate initial/boundary values. Here, we approach in particular the equations for velocity.

The performance of the most common methods depends greatly on the flow formulation that they assume. On solving the model in primitive variables, several methods meet the equation for the mass conservation by cumbersome iterative precedures that solve the related Poisson equation for pressure. This approach allows a straightforward assignement of the boundary values but the residual compressibility may affect the transient regime. The computation of pressure is avoided by solving the vorticity transport equation. In this case the model in velocity and vorticity still presents the same peculiarities. The models in vector potential functions provide exactly solenoidal velocity fields (at least for confined flows) but they incur in a complicated formulation of the boundary conditions, which is still not clear for general domains (e.g. multiple connection).

These characteristics are even more evident within a domain decomposition approach because they result in a combined effect for the computations in each subdomain.

We solve the equations for the vector potential via domain decomposition on accepting boundary/interface conditions directly in primitive variables. By an algebraic rearrangement of the discrete equations for velocity and pressure in a neighborhood of the boundary/interface, we determine conditions that combined to the discrete equations for the vector potential define uniquely the flow in each subdomain. The solutions are exactly mass conserving at each time step like in the case of the classical vector potential formulation but the mentioned limitation of this model in the assignement of the boundary conditions is overcome as they are directly and easily adopted from the physical application.

2. Domain decomposition for the MDVP model

We decompose the flow domain into slices parallel to a wall of the cavity. In each subdomain, the MDVP model is adopted. This is based on a modification of the discrete vector potential model (DVP) that is described in detail in [1]. In the following we outline the method.

For the sake of semplicity in the exposition, it is convenient to recall the main steps of the DVP numerical formulation. Let us indicate with $\mathbf{w}^m, \mathbf{p}^m$ respectively the discrete velocity and the discrete pressure vectors for the generic subdomain, which are assigned on a regular MAC–like staggered grid, [3]; let us assume that

$$\begin{aligned} &Q_m \mathbf{w}^m = -A^T \mathbf{p} + \mathbf{b}_m \\ &A\mathbf{w} = 0 \end{aligned} \tag{2}$$

be the matricial form of the finite difference discretization of the momentum and mass equations $(1^{'}.1^{'''})$ at time level t_m; Q_m be the matrix of the temporal, convective and diffusive discrete terms; $\mathbf{b}_m$ be the vector of the body force and boundary effects; $\mathbf{s}_m$ be the vector of the discrete boundary normal velocity; A

and A^T be respectively the centred difference divergence and gradient operator (for the rank(A) see [1]).

It is known that the solution of the system of linear equations $(2'')$ may be split into a particular solution, $\mathbf{y}^m$, and the general solution of the related homogeneous system, $\mathbf{z}^m$, that is:

$$\mathbf{w}^m = \mathbf{y}^m + \mathbf{z}^m. \tag{3}$$

As it is possible to build a network representing the relations assignement point/variable in the adopted discretization grid [1], from network theory we get the expression of a matrix C (foundamental matrix) whose column vectors form a basis of the kernel(A), which the velocity field $\mathbf{z}^m$ belongs to. It holds:

$$AC = 0, C^T A^T = 0, \mathbf{z}^m = C\gamma^m, \tag{4}$$

where γ^m is the vector of the new velocity components.

From network theory we learn also an easy and exact expression for a particular solution, $\mathbf{y}^m$, (spanning tree).

By combining (3) and (4) into $(2')$ and rearranging, the system which is finally solved is obtained:

$$C^T Q_m C\gamma^m = C^T(\mathbf{b}_m - Q^m \mathbf{y}^m). \tag{5}$$

Regardless the accuracy of the solution γ^m of (5), by $(4''')$ it results that the correspondent velocity $\mathbf{w}^m$ satisfies exactly $(2'')$. Actually, it is shown that γ^m is a discrete vector potential field, C and C^T are both centred difference curl operators, and the discrete model (5) is just a discrete form of the vorticity transport equation for a vector potential.

The MDVP method stems from this remark and is justified by the fact that the computation of the product matrix in (5) is more time consuming than the determination of the solution of the system.

We avoid the computation of the whole product matrix by discretizing directly the equations for the vector potential in the internal mesh points and completing the system with those equations from (5) that recall the boundary/interface values.

We adopt the decomposition of the velocity vector field suggested by the DVP model (see (3) and (4"'))

$$\mathbf{w} = \mathbf{y} + \nabla \wedge \gamma \tag{6}$$

being $\mathbf{y}$, a solenoidal vector field and γ, a vector potential field. This is analogous to the modified Helmoltz decomposition presented in [4].

The vector $\mathbf{y}$ is discretized at the velocity grid points; it is computed in the way indicated within the DVP model, that is in order to meet exactly the boundary normal velocity values and the divergence–free condition on $\mathbf{w}$.

The vector potential field γ is chosen to be a 3D regular vector field having null boundary/interface tangential components and, in the interior of the

domain, one component zero everywhere except at any fixed normal coordinate plane. This restriction allows as well the representation of any Navier–Stokes flow field as it is recovered directly by the DVP model (structure of the vector γ^m and the matrix C). γ is determined by the following vorticity transport equation:

$$\begin{aligned} &\tfrac{1}{\sqrt{Gr}}\tfrac{\partial(\nabla\wedge(\mathbf{y}+\nabla\wedge\gamma))}{\partial t}+((\mathbf{y}+\nabla\wedge\gamma)\cdot\nabla)(\nabla\wedge(\mathbf{y}+\nabla\wedge\gamma))- \\ &\qquad((\nabla\wedge(\mathbf{y}+\nabla\wedge\gamma))\cdot\nabla)(\mathbf{y}+\nabla\wedge\gamma)= \\ &\qquad\tfrac{1}{\sqrt{Gr}}\nabla^2(\nabla\wedge(\mathbf{y}+\nabla\wedge\gamma))-\nabla\wedge\tfrac{\mathbf{g}}{|\mathbf{g}|}T. \end{aligned} \tag{7}$$

We discretize the above equation by using centred finite differences for the curl operator and the same schemes adopted within the DVP model for the time derivative, the convective and the diffusive terms. Then, γ is assigned on the staggered grid obtained by drawing lines that connect the discrete pressure points along the directions of the discrete velocity values.

Close to the boundary/interface, where boundary/interface values intervene in the discrete system, we substitute locally the discrete curl of the discrete momentum equation in primitive variables in order to accept the boundary/interface values of the velocity and pressure fields. The discrete velocity values that fall in the interior of the domain are still expressed according to the decomposition (6). In this way the overall discrete system that we build, in each subdomain results in being same of system (5) but we have avoided the cumbersome computation of the matrix product C^TQ_mC.

We have previously experienced domain decomposition for the DVP method and reported our experience in [6], [7]. There we have reached the conclusion that the capacitance matrix method is certainly the most efficent and accurate, once a direct solver for the capacitance system is available. Unfortunately, in our case the structure of this system is very complicated and its matrix has a very large band so that a direct procedure is indeed too costly. As by an iterative solver (Jacoby, Gauss–Siedel, ..) this method results totally equivalent to a Schwarz method, we follow directly the overlapping Schwarz multiplicative method: calculations are carried out by sweeping the entire domain from the first to the last "slice"; the flow is computed at one subdomain at a time by assuming the last updated values at the interfaces. Interface conditions are expressed in velocity and treated like general boundary conditions. In order to start up domain decomposition iterations, a preconditioner based on a multigrid type method is used so as to avoid the growth of spourious flow microstructures in the interface regions: the initial iterate is computed twice with double spacing for the first approximation. At the moment for the solution of the system (5) a squared conjugated gradient method is used but along the lines traced in [5], we are studying a more specific and efficient approach.

3. Numerical results

For the following tests, we divide the domain into four subdomains overlapping along a mesh band two-cells large. The mesh size is $34 \times 34 \times 34$.

We checked the accuracy of the overall computational procedure running the Taylor analytical 2D flow. The velocity components are the following: $u = \sin \pi x \cos \pi z \exp(-2t/\text{ Re})$, $v = -\cos \pi x \sin \pi z \exp(-2t/\text{ Re})$, [1]. We solved the flow at Re $= 1$ in a cubic cavity with unitary side length by imposing the analytical velocity values at the boundaries.

The results, that we obtained with $\Delta t = 0.001$, exibit an average relative error equal to 0.001 at the first five time steps.

Then we computed the classical "driven cavity" flow problem: a fluid at rest in a cubic cavity with rigid walls, is induced to recirculate for the viscosity by an ideal infinite lateral lid which moves at constant unitary velocity. We considered the cases at Re $= 1$ and Re $= 400$ and compared the results with the solutions by the DVP model for 1–domain: this agreement is up to the fifth significant digit. As the flow is symmetric we ran the computation in half cavity. In **fig. 1** we plot the isovorticity surfaces at Re $= 400$ for the transient solution computed with $\Delta t = 0.01$ at the 640–th time step (this is very close to the steady state). In the table are listed the number of domain decomposition iterations vs. the time step.

# DD iter.	13	10	8	6	4	3	3	2	1	1	1
time step	1	2	3	5	7	9	11	13	15	...	640

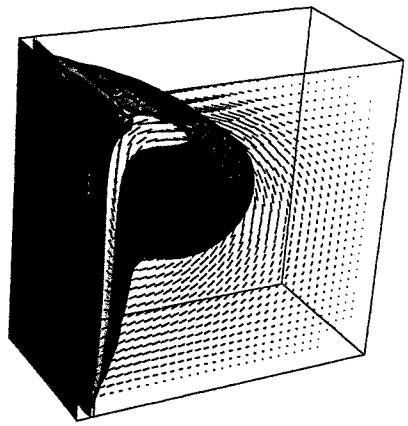

Fig. 1

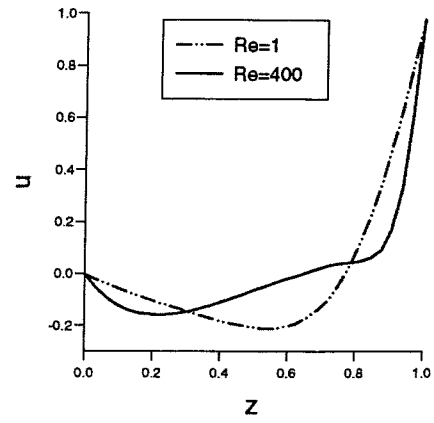

Fig. 2

In **fig. 2** there are the profiles of the velocity component parallel to the driving direction, u, along the orthogonal central line for the steady state. In **fig. 3** the same profile at Re $= 400$ is plotted as the horizontal coordinate y varies, from the middle plane parallel to the primary vortex back to the impermeable wall.

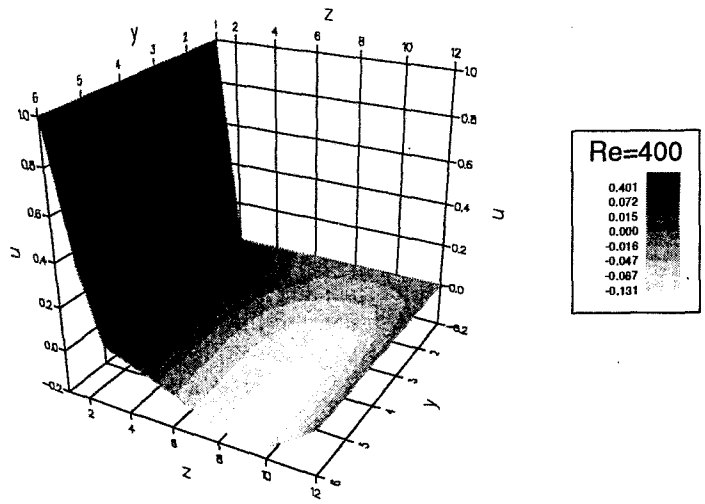

Fig. 3

Acknowledgements. We are grateful to Prof. R. Piva and Prof. G. Graziani for the useful discussions. We thank Prof. P. Orlandi for providing us with 3D flow plotting routines.

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