Numerical Simulation of Three-Dimensional Viscous Flows using the Vector Potential Method*

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A method for solving three-dimensional viscous incompressible flows is presented. A complete set of the Navier-Stokes equation is transferred and expressed in terms of the vorticity, the scalar and the vector potential. In this formulation, the velocity field satisfies the equation of continuity automatically. The vorticity transport equations discretized by the centered differences are solved by the rational Runge-Kutta (RRK) time integration scheme, and the Poisson equations are solved by the successive over-relaxation (SOR) method. The numerical solutions of flows in a cubic cavity, in a square duct and in a rectangular duct with the aspect ratio of 2 are presented. Comparison of computed results with other calculations confirms the accuracy and reliability of the present approach.

Key Words: Computational Fluid Dynamics, Finite Difference Method, Three-Dimensional Flow, Internal Flow, Duct Flow, Secondary Flow

1. Introduction

Efficient computational methods are needed for three-dimensional incompressible flows from the practical point of view. The three-dimensional Navier-Stokes equations have been solved so far in the primitive variables formulation. It is, however, difficult to satisfy the equation of continuity in this method.

In two-dimensional flows the vorticity-stream function formulation is often used. On three-dimensional flows, however, the vector potential ϕ is introduced from $\mathbf{u} = \nabla \times \phi$ where $\mathbf{u}$ denotes the velocity field. Then, the Navier-Stokes equations are transformed into the vorticity transport equations for the vorticity $\xi = \nabla \times \mathbf{u}$, and the Poisson equations are defined for the vector potential ϕ . In this formulation, the equation of continuity is automatically satisfied so that the present method is expected to be an efficient computational method for solving incompressible

flows.

The cubic cavity flow is at first computed by the present method at the Reynolds numbers 100 and 400. Computational results are compared with calculations using the primitive variables formulation and the pseudospectral method in order to examine the accuracy and reliability of the present method. The three-dimensional computational method is also applied to calculations of flows in straight ducts with a square and a rectangular cross section.

2. Governing Equations and Computational Methods

2.1 Governing equations

Three-dimensional motions of fluid are described by the Navier-Stokes equations and the equation of continuity:

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla p + \frac{1}{Re} \nabla^2 \mathbf{u}, \quad (1)$$

$$\nabla \cdot \mathbf{u} = 0, \quad (2)$$

where p is the pressure and Re is the Reynolds number. These equations are normalized with the representative length and velocity. Now we define the

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vorticity $\xi = (\xi_x, \xi_y, \xi_z)$ as

$$\xi = \nabla \times \mathbf{u}. \quad (3)$$

Then, the Navier-Stokes equations (1) are transformed into the vorticity transport equations with the conservative form:

$$\frac{\partial \xi_x}{\partial t} = -\nabla \cdot (\mathbf{u} \xi_x) + (\xi \cdot \nabla) u + \frac{1}{Re} \nabla^2 \xi_x, \quad (4)$$

$$\frac{\partial \xi_y}{\partial t} = -\nabla \cdot (\mathbf{u} \xi_y) + (\xi \cdot \nabla) v + \frac{1}{Re} \nabla^2 \xi_y, \quad (5)$$

$$\frac{\partial \xi_z}{\partial t} = -\nabla \cdot (\mathbf{u} \xi_z) + (\xi \cdot \nabla) w + \frac{1}{Re} \nabla^2 \xi_z. \quad (6)$$

On the other hand, the vorticity field $\mathbf{u}$ is represented in terms of the vector potential $\phi = (\phi_x, \phi_y, \phi_z)$ and the scalar potential ϕ as

$$\mathbf{u} = \nabla \times \phi + \nabla \phi. \quad (7)$$

The Laplace equation is derived from the substitution of Eq. (7) into (2) and the usage of the relation $\nabla \cdot (\nabla \times \phi) = 0$

$$\nabla^2 \phi = 0. \quad (8)$$

The relationship between ϕ and ξ is derived from the rotation of Eq. (7):

$$\nabla (\nabla \cdot \phi) - \nabla^2 \phi = \xi. \quad (9)$$

In Eq. (9), we assume the solenoidal condition represented as

$$\nabla \cdot \phi = 0. \quad (10)$$

Finally, the three-dimensional Poisson equations yield for the vector potential as follows:

$$\nabla^2 \phi = -\xi. \quad (11)$$

Since the flow in a cubic cavity closes, the velocity is represented as

$$\mathbf{u} = \nabla \times \phi. \quad (12)$$

In duct flows, however, we must replace $\nabla \phi$ in Eq. (7) to the inflow velocity (0, 0, 1). The velocity, is, therefore, represented by

$$\mathbf{u} = \nabla \times \phi + (0, 0, 1). \quad (13)$$

2.2 Numerical method for the vorticity transport equations

The method of lines is adopted in the present investigation. In this method, spatial discretizations and the time integration are treated separately. For spatial discretizations the centered difference method is used. For instance, partial derivatives in the x -direction of ξ are approximated at the grid point (i, j, k) according to the following expressions:

$$\frac{\partial \xi}{\partial x} \bigg|_{ijk} = \frac{\xi_{i+1,j,k} - \xi_{i-1,j,k}}{2\Delta x}, \quad (14)$$

$$\frac{\partial^2 \xi}{\partial x^2} \bigg|_{ijk} = \frac{\xi_{i+1,j,k} - 2\xi_{i,j,k} + \xi_{i-1,j,k}}{\Delta x^2}, \quad (15)$$

where Δx is the grid spacing in the x -direction. The same discretizations are yielded for derivatives in the y - and z -directions. After spatial discretizations, the partial differential equations are reduced to a set of ordinary differential equations for the vorticity values at inner grid points.

$$\frac{d\vec{\xi}}{dt} = \vec{F}(\vec{\xi}), \quad (16)$$

$$\vec{\xi} = (\xi_{x,2,2,2}, \xi_{x,3,2,2}, \dots, \xi_{x,I-1,J-1,K-1})^T. \quad (17)$$

In Eq. (17) I, J and K represent the total grid points in the x -, y - and z - directions, respectively.

Although a number of integration methods are applicable to Eq. (16) with Eq. (17), stability of classical explicit methods is restricted strictly. In the present study, therefore, we use the RRK method which is proposed by Wambec⁽¹⁾ and shown to be unconditionally stable for the single equation. This method is composed of two steps such that

$$\vec{\xi}^{(1)} = \vec{\xi}^{(n)} + c_2 \vec{g}_1, \quad \vec{g}_1 = \Delta t \vec{F}(\vec{\xi}^{(n)}), \quad (18)$$

$$\vec{\xi}^{(n+1)} = \vec{\xi}^{(n)} + \frac{2\vec{g}_1(\vec{g}_1, \vec{g}_3) - \vec{g}_3(\vec{g}_1, \vec{g}_1)}{(\vec{g}_3, \vec{g}_3)}, \quad (19)$$

$$\vec{g}_2 = \Delta t \vec{F}(\vec{\xi}^{(1)}), \quad \vec{g}_3 = b_1 \vec{g}_1 + b_2 \vec{g}_2, \quad (20)$$

where $(\vec{d}, \vec{e})$ represents a scalar product between the vector $\vec{d}$ and $\vec{e}$. The numerical constants b_1, b_2 and c_2 are specified adequately, and the second-order accuracy is assured for $b_2 c_2 = -1/2$.

2.3 Numerical method for the Poisson equations

The Poisson equations are solved by the SOR method. Spatial discretizations are carried out in terms of the centered difference. Solving discretized equations with respect to ϕ_{ijk} , we obtain

$$\phi_{ijk} = \frac{1}{2(1 + \beta_1^2 + \beta_2^2)} \times \{ (\phi_{i+1,j,k} + \phi_{i-1,j,k}) + \beta_1^2 (\phi_{i,j+1,k} + \phi_{i,j-1,k}) + \beta_2^2 (\phi_{i,j,k+1} + \phi_{i,j,k-1}) + \Delta x^2 \xi_{ijk} \}, \quad (21)$$

where $\beta_1 = \Delta x / \Delta y$ and $\beta_2 = \Delta x / \Delta z$. The vector potentials at the $(n+1)$ -th relaxation step ϕ_{ijk}^{n+1} are specified by adding $0 = \phi_{ijk}^n - \phi_{ijk}^n$ to Eq. (21) and introducing the acceleration factor ω ,

$$\phi_{ijk}^{n+1} = \phi_{ijk}^n + \frac{\omega}{2(1 + \beta_1^2 + \beta_2^2)} \times \{ (\phi_{i+1,j,k}^n + \phi_{i-1,j,k}^n) + \beta_1^2 (\phi_{i,j+1,k}^n + \phi_{i,j-1,k}^n) + \beta_2^2 (\phi_{i,j,k+1}^n + \phi_{i,j,k-1}^n) + \Delta x^2 \xi_{ijk} - 2(1 + \beta_1^2 + \beta_2^2) \phi_{ijk}^n \}. \quad (22)$$

In the present calculations we adopt $\omega = 1.5$.

3. Calculations of Cubic Cavity Flow

3.1 Computational conditions

We consider a cubic cavity, with the unit length, where the plane at $y=1$ moves in the z -direction with the unit velocity, as shown in Fig. 1. At the initial instant we assume $\mathbf{u}=0, \phi=0$ and $\xi=0$ at the computational domain.

3.2 Boundary conditions

The no-slip boundary condition is applied to six walls at the cubic cavity. The vector potential and the vorticity are, therefore, specified by the following conditions.

3.2.1 Boundary conditions for ϕ Tangential components of ϕ to the wall vanish and the normal

derivative is specified as zero with respect to the normal component. On the walls of $x=0$ and 1 , for example, we impose

$$\frac{\partial \psi_x}{\partial x} = \psi_y = \psi_z = 0. \quad (23)$$

3.2.2 Boundary conditions for ζ The vorticity on the wall is expressed from its definition. On walls of $x=0$ and 1 , we impose

$$\zeta_x = 0, \zeta_y = -\frac{\partial w}{\partial x}, \zeta_z = \frac{\partial u}{\partial x}. \quad (24)$$

3.3 Results

The uniform grid is used in the x -, y -, and z -directions. The number of grid points is taken as 21^3 at $Re=100$ and 31^3 at $Re=400$. Figure 2 depicts the velocity profile of w on the line $x=z=0.5$. The present result is compared with the calculations of Takami and Kuwahara⁽²⁾, Goda⁽³⁾, and Ku et al.⁽⁴⁾ The present result shows the best agreement with the calculation of Ku et al. using the pseudospectral method at $Re=100$. Its tendency becomes more remarkable at $Re=400$. The grid 31^3 is needed in the present calculation because we use the uniform grid from the viewpoint of simplicity. The same result is probably obtained in terms of fewer grid points when we use the nonuniform mesh. The computation of Ku et al. is carried out in the half region at the cubic cavity using $13 \times 25 \times 25$ mesh.

The solenoidal condition(10) is assumed on deriving the Poisson equations for the vector potential(11). It is crucially important whether this condition is satisfied in actual computations. Table 1 shows root mean squares of $\nabla(\nabla \cdot \phi)$ and $\Delta \phi$ for the present computational results. The ratio between root mean squares $\nabla(\nabla \cdot \phi)$ and $\Delta \phi$ increases with the Reynolds number and decreases with the number of grid points. The satisfaction of the solenoidal condition is, however, assured within 7 percent at $Re=100$ and 9 percent at $Re=400$.

The velocity profile in the plane $z=0.5$ is depicted in Fig. 3. The boundary layer is formed at both the moving and depth wall at $Re=400$, while the velocity

Fig. 1 3D driven cavity

changes gradually at $Re=100$. We show the velocity vector plots on the planes $x=0.5$ and $z=0.5$ in Figs. 4 and 5, respectively. It is found that the center of the vorticity displaces to the bottom as the Reynolds number increases. A pair of vortices is seen to be captured from Fig. 5. The vortex pair also moves downward with increasing Reynolds number, and the secondary vortices are formed in the vicinity of the moving wall. The magnitude of the velocity vectors in Fig. 5 is strengthened to 1.5 times compared with that in Fig. 4.

(a) $Re=100$

(b) $Re=400$

Fig. 2 Profile of the driven component velocity w along the central vertical line

Table 1 Comparison between root mean squares $\nabla(\nabla \cdot \phi)$ and $\Delta \phi$

Grid Points	Re		x-Component	y-Component	z-Component
9 × 9 × 9	1	$\nabla(\nabla \cdot \phi)$	0.02843	0.02379	0.01471
		$\Delta \phi$	1.59569	0.20066	0.19103
		$\nabla(\nabla \cdot \phi)/\Delta \phi$	0.0178	0.118	0.0770
	50	$\nabla(\nabla \cdot \phi)$	0.03305	0.02958	0.02527
		$\Delta \phi$	1.54996	0.23610	0.24527
		$\nabla(\nabla \cdot \phi)/\Delta \phi$	0.0213	0.125	0.103
	100	$\nabla(\nabla \cdot \phi)$	0.09878	0.07468	0.08030
		$\Delta \phi$	1.45636	0.38297	0.42918
		$\nabla(\nabla \cdot \phi)/\Delta \phi$	0.0678	0.195	0.187
21 × 21 × 21	100	$\nabla(\nabla \cdot \phi)$	0.03592	0.02889	0.18438
		$\Delta \phi$	2.35569	0.44330	0.40361
		$\nabla(\nabla \cdot \phi)/\Delta \phi$	0.0152	0.0651	0.0456
31 × 31 × 31	400	$\nabla(\nabla \cdot \phi)$	0.08359	0.06014	0.05928
		$\Delta \phi$	2.70777	0.70227	0.67780
		$\nabla(\nabla \cdot \phi)/\Delta \phi$	0.0308	0.0856	0.0874

Fig. 3 Profile of the driven component velocity w in the plane $z=0.5$

Fig. 4 Velocity vector plots in the plane $x=0.5$

Fig. 5 Velocity vector plots in the plane $z=0.5$

Fig. 6 Straight duct

4. Calculations of Duct Flows with Square and Rectangular Cross Section

4.1 Computational conditions

Now we calculate duct flows with a square and a rectangular cross section shown in Fig. 6. In the duct with the rectangular cross section, the aspect ratio is taken as 2. The Reynolds number is defined, in this case, as $Re = w_0 D / \nu$ by the hydraulic diameter D , the inflow velocity w_0 and the kinematic viscosity ν . The computations are carried out from the normalized length $(z/D)/Re = 0$ to 0.1. We use the grid $13 \times 13 \times 41$ for the square duct and $13 \times 25 \times 41$ for the rectangular duct, respectively. The initial condition is specified in terms of $u = (0, 0, 1)$, $\phi = 0$ and $\zeta = 0$ at the full region.

4.2 Boundary conditions

An axial flow with the unit strength is assumed in the plane $z=0$.

4.2.1 Boundary conditions for ϕ At the inlet we adopt conditions

$$\phi_x = \phi_y = \frac{\partial \phi_z}{\partial z} = 0. \quad (25)$$

At the outlet, we assume that the normal derivatives of the tangential components vanish:

$$\frac{\partial \phi_x}{\partial z} = \frac{\partial \phi_y}{\partial z} = 0. \quad (26)$$

From the solenoidal condition the normal component is specified as

$$\frac{\partial \psi_z}{\partial z} = -\frac{\partial \psi_x}{\partial x} - \frac{\partial \psi_y}{\partial y}. \quad (27)$$

4.2.2 Boundary conditions for ζ The vorticity is calculated at the inlet

$$\zeta_x = -\frac{\partial v}{\partial z}, \quad \zeta_y = \frac{\partial u}{\partial z}, \quad \zeta_z = 0. \quad (28)$$

At the outlet, however, we assume

$$\frac{\partial \zeta_x}{\partial z} = \frac{\partial \zeta_y}{\partial z} = \zeta_z = 0. \quad (29)$$

For wall boundary conditions, we use the same conditions applied to calculations of the cubic cavity flow.

4.3 Results

The velocity profile in the square duct is depicted at the normalized distance $(z/D)/Re = 0.0075, 0.02$ and 0.1 in Fig. 7. The maximum velocity increases with the normalized distance and develops. The result is compared with calculations using the PNS and PPNS equation. Although the flow development is retarded in comparison with other results, the concavity in the velocity profile is predicted as the result of the PPNS. The fully developed flow, however, agrees excellently with other results, and w/w_0 reaches 2.11 at the center line. Figure 8 shows the velocity vector plots on the plane $(z/D)/Re = 0.0075$. It depicts how the secondary flow is raised from the wall to the central direction in order to develop the flow. The secondary flow results in the increase of the center velocity.

The velocity profile is depicted for the duct flow with the rectangular cross section of the aspect ratio 2 in Fig. 9. The velocity profile at the normalized distance $(z/D)/Re = 0.0038$ shows the off-center maxima, which has the same tendency as the square duct flow. As the flow develops, the maximum velocity reaches 1.99, while the distribution differs significantly between on the line $x=0$ and $y=0$. We show the velocity vector plots of the secondary flow at $(z/D)/Re = 0.0075$ in Fig. 10. The flow velocity is larger in the y -direction than in the x -direction, which is the straightforward consequence of the rectangular duct.

Fig. 7 Normalized transverse distance versus axial velocity ratio w/w_0

Fig. 8 Velocity vector plots in the cross section $(z/D)/Re = 0.0075$

(a) $x/L=0$ plane

(b) $y/H=0$ plane

Fig. 9 Normalized transverse distances vs axial velocity ratio w/w_0

Fig. 10 Velocity vector plots in the cross section $(z/D)/Re = 0.0075$

5. Conclusions

A numerical algorithm is proposed for calculating viscous incompressible internal flows. The vector potential formulation is adopted, and the RRK method is used for the time integration of the vorticity transport equations. The Poisson equations are solved for the vector potentials. The present method is applied to calculations of cubic cavity flows as well as the duct flows with the square and rectangular cross section. From the present calculations, the following conclusions are obtained:

- (1) The present method gives the same results as the pseudospectral method for the cubic cavity flows at the Reynolds numbers 100 and 400.
- (2) For duct flows with the square and the rectangular cross section (the aspect ratio 2), the present results not only predict the concavity in the inlet velocity profile but also agree excellently with other results with respect to fully developed flow.

It is demonstrated from the above results that the

present method is accurate and efficient for calculating viscous incompressible flow.

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