High-Accuracy Analysis of Three-Dimensional Advection Equation Using Finite Difference Methods*

Shinji KAWAMOTO**, Hirohiko IWASE***
and Takahiko TANAHASHI***

Instability of numerical flow analysis at high Reynolds number is caused by spurious high-wave-number oscillations which are produced by the convection term of the Navier-Stokes equation. To correct the instability, some finite difference methods for the convection term have been proposed, such as the QUICK method, the QUICKEST method and the third-order upwind difference method. In this paper, the stability and accuracy of typical finite difference methods, i.e., the 2nd-order centered difference method, the QUICK method, the 3rd-order upwind difference method, the QUICKEST method, the 4th-order centered difference method, the 5th-order upwind difference method and the 6th-order centered difference method, are evaluated by computing the three-dimensional advection equation, i.e., the rotating sphere problem. The 3rd-order Adams-Bashforth method is mainly applied as a time integration method.

Key Words: Computational Fluid Dynamics, Numerical Analysis, Finite Difference Method, Rotating Cone, Rotating Sphere, Advection Equation, Three-Dimensional Flow

1. Introduction

Flow analysis at high Reynolds number is an interesting problem in engineering. In flow analysis, numerical instability is caused by spurious high-wave-number oscillations which are produced by the convection term of the Navier-Stokes equation. Therefore the finite difference method for the convection term is significant in numerical analysis.

When the convection term is discretized by the centered difference method, the numerical solution contains high-wave-number oscillations which are produced by the major term of the truncation error, i.e., the odd-order differential term. The upwind difference methods improve the instability, but when the convection term is discretized by the 1st-order upwind difference method, the major term of the

truncation error becomes a 2nd-order differential term which is of the same order as the physical diffusion term. Hence this artificial viscosity impairs the accuracy severely when the convection is dominant. Kawamura and Kuwahara proposed a 3rd-order upwind difference method in which the major truncation error is of the 4th-order⁽¹⁾. Even though the truncation error is of a higher order than the physical diffusion term, the even-order truncation error works as the artificial viscosity.

Matsushita et al.⁽²⁾ studied the stability and accuracy of the 3rd-order upwind difference method by computing a one-dimensional advection equation. After that, Okanaga et al.⁽³⁾ studied the stability and accuracy of typical finite difference methods by computing a two-dimensional advection equation.

In this paper, the stability and accuracy of the typical finite difference methods, i.e. the 2nd-order centered difference method, the QUICK method⁽⁴⁾, the 3rd-order upwind difference method, the QUICKEST method⁽⁵⁾, the 4th-order centered difference method, the 5th-order upwind difference method and the 6th-order centered difference method, are evaluated by computing a three-dimensional advection equation,

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** Production and Technical Department, Nippon Sheet Glass Co., Ltd., 6, Anesakikaigan, Ichihara, Chiba 299-01, Japan

*** Department of Mechanical Engineering, Keio University, 3-14-1, Hiyoshi, Kohoku-ku, Yokohama 223, Japan

i.e., the rotating sphere problem. The 2nd-order Adams-Bashforth method and the 3rd-order Adams-Bashforth method are applied as time integration methods.

2. Basic equations

The advection equation is described by

$$\frac{\partial \phi}{\partial t} = f(\phi), \quad (1)$$

where

$$f(\phi) = -u \frac{\partial \phi}{\partial x} - v \frac{\partial \phi}{\partial y} - w \frac{\partial \phi}{\partial z}. \quad (2)$$

Here, u , v and w are the given flow velocity components, and ϕ is the scalar potential. We used two kinds of time integration methods, i.e., the 2nd-order Adams-Bashforth method

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = \frac{3f(\phi^n) - f(\phi^{n-1})}{2}, \quad (3)$$

and the 3rd-order Adams-Bashforth method

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = \frac{23f(\phi^n) - 16f(\phi^{n-1}) + 5f(\phi^{n-2})}{12}, \quad (4)$$

as time integration methods.

We evaluated typical finite difference methods, i.e., the 2nd-order centered difference method, the QUICK method, the 3rd-order upwind difference method, the QUICKEST method, the 4th-order center-

ed difference method, the 5th-order upwind difference method and the 6th-order centered difference method. Table 1 shows x -component of each spatial discretization method. The QUICKEST method, developed by Leonard⁽⁶⁾, is the 3rd-order discretization method for space and time. The discretized x -component of the QUICKEST method is written as follows for $u > 0$.

$$\begin{aligned} \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = & -u_i \frac{2\phi_{i+1}^n + 3\phi_i^n - 6\phi_{i-1}^n + \phi_{i-2}^n}{2\Delta x} \\ & + u_i^2 \frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{2\Delta x^2} \Delta t \\ & - u_i^3 \frac{\phi_{i+1}^n - 3\phi_i^n + 3\phi_{i-1}^n - \phi_{i-2}^n}{6\Delta x^3} \Delta t^2 \\ & + \frac{u_i}{12} \frac{\partial^4 \phi}{\partial x^4} \Big|_i \Delta x^3 + \frac{1}{24} \frac{\partial^4 \phi}{\partial t^4} \Big|_n \Delta t^3 + O(\Delta t^4, \Delta x^4) \end{aligned} \quad (5)$$

3. Numerical model

The advection equation contains no diffusion term. Therefore when the velocity is set for flow as a rigid rotation in the analysis area, the initial scalar potential flows without transformation. Figure 1 shows the analysis model. The analysis area is a cube in which the length of one side is 2. The flow is rigid rotation on the z' -axis. The angle formed by the z -axis and the z' -axis is θ . When $\theta = 0$, w becomes 0.

Table 1 Spatial discretization methods

2nd-order centered difference method	$u \frac{\partial \phi}{\partial x} \Big _i = u_i \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} - \frac{u_i}{6} \frac{\partial^3 \phi}{\partial x^3} \Big _i \Delta x^2 + O(\Delta x^3)$
QUICK method	$\begin{aligned} u > 0 \\ u \frac{\partial \phi}{\partial x} \Big _i = & u_i \frac{3\phi_{i+1} + 3\phi_i - 7\phi_{i-1} + \phi_{i-2}}{8\Delta x} - \frac{u_i}{24} \frac{\partial^3 \phi}{\partial x^3} \Big _i \Delta x^2 \\ & + \frac{u_i}{16} \frac{\partial^4 \phi}{\partial x^4} \Big _i \Delta x^3 + O(\Delta x^4) \end{aligned}$
3rd-order upwind difference method	$\begin{aligned} u \frac{\partial \phi}{\partial x} \Big _i = & u_i \frac{-\phi_{i+2} + 8\phi_{i+1} - 8\phi_{i-1} + \phi_{i-2}}{12\Delta x} \\ & + \alpha u_i \frac{\phi_{i+2} - 4\phi_{i+1} + 6\phi_i - 4\phi_{i-1} + \phi_{i-2}}{12\Delta x} - \alpha \frac{ u_i }{12} \frac{\partial^4 \phi}{\partial x^4} \Big _i \Delta x^3 + O(\Delta x^4) \end{aligned}$
4th-order centered difference method	$u \frac{\partial \phi}{\partial x} \Big _i = u_i \frac{-\phi_{i+2} + 8\phi_{i+1} - 8\phi_{i-1} + \phi_{i-2}}{12\Delta x} + \frac{u_i}{30} \frac{\partial^5 \phi}{\partial x^5} \Big _i \Delta x^4 + O(\Delta x^5)$
5th-order upwind difference method	$\begin{aligned} u \frac{\partial \phi}{\partial x} \Big _i = & u_i \frac{\phi_{i+3} - 9\phi_{i+2} + 45\phi_{i+1} - 45\phi_{i-1} + 9\phi_{i-2} - \phi_{i-3}}{60\Delta x} \\ & + \alpha u_i \frac{-\phi_{i+3} + 6\phi_{i+2} - 15\phi_{i+1} + 20\phi_i - 15\phi_{i-1} + 6\phi_{i-2} - \phi_{i-3}}{60\Delta x} \\ & + \alpha \frac{ u_i }{60} \frac{\partial^6 \phi}{\partial x^6} \Big _i \Delta x^5 + O(\Delta x^6) \end{aligned}$
6th-order centered difference method	$\begin{aligned} u \frac{\partial \phi}{\partial x} \Big _i = & u_i \frac{\phi_{i+3} - 9\phi_{i+2} + 45\phi_{i+1} - 45\phi_{i-1} + 9\phi_{i-2} - \phi_{i-3}}{60\Delta x} \\ & - \frac{u_i}{140} \frac{\partial^7 \phi}{\partial x^7} \Big _i \Delta x^6 + O(\Delta x^7) \end{aligned}$

Fig. 1 Rotating sphere model

Hence the numerical results are equivalent to the results in the two-dimensional problem when $\theta=0$. The initial condition of scalar potential ϕ is given by

$$\left. \begin{aligned} \phi &= \frac{\cos(\pi r/0.3)+1}{2} & (r < 0.3) \\ \phi &= 0 & (r \geq 0.3) \end{aligned} \right\} \quad (6)$$

Where r is the distance from the center of the potential sphere $(0, 0.5, 0)$.

The accuracy of the computations is evaluated by the maximum value of the scalar potential and root mean square error at time $t=2\pi$, when the potential makes a round. The root mean square error is written as

$$E = \left(\sum_{i=1}^N (\phi_{ni} - \phi_{ei})^2 \right) / N \quad (7)$$

Where ϕ_e is the theoretical result, which is the initial condition, ϕ_n is the numerical result, and N is the

Initial Condition

(a) Potential contours
(red : $\phi=0.01$, yellow : $\phi=0.5$)

(a) Potential contours
(red : $\phi=0.01$, yellow : $\phi=0.5$)

(b) Potential elevations on cross sections
Fig. 2 Initial condition

(b) Potential elevations on cross sections
Fig. 3 Potential after one rotation
(by QUICK method)

node number.

4. Numerical results and discussion

Figures 2(a) and 2(b) show the initial condition of potential ϕ . Figure 2(a) shows the potential contour, i.e., $\phi=0.01$ on the red surface and $\phi=0.5$ on the yellow surface. Figure 2(b) shows the potential elevation on cross sections which pass the center of the potential sphere, i.e., x -plane($x=0$), y -plane($y=0.5$), z -plane($z=0$).

Figures 3 to 8 show the numerical results for 27 000 uniform mesh, $\theta=45^\circ$ and $\Delta t=0.01$ (the Courant number at the center of the potential sphere is 0.15).

In this case, the 3rd-order Adams-Bashforth method is applied as the time integration method. Comparing these results with initial conditions, we

can visually evaluate the accuracy of each finite difference method.

Table 2 shows the maximum value of the potential $\phi_{\max}$ and Fig. 9 shows the mean square error E after one rotation for $\theta=0^\circ$ to 45° .

The QUICKEST method and the 3rd-order upwind difference method are 3rd-order spatial discretization methods. Therefore, $\phi_{\max}$ and E of these

Table 2 Maximum value of ϕ after one rotation

	$\theta = 0^\circ$	$\theta = 15^\circ$	$\theta = 30^\circ$	$\theta = 45^\circ$
QUICK	0.664	0.613	0.577	0.577
3rd-order upwind ($\alpha = 1$)	0.631	0.572	0.540	0.532
QUICKEST	0.628	0.565	0.535	0.532
4th-order centered	0.928	0.932	0.923	0.929
5th-order upwind ($\alpha = 1$)	0.895	0.889	0.879	0.876
6th-order centered	0.989	0.999	1.016	1.020

(a) Potential contours
(red : $\phi=0.01$, yellow : $\phi=0.5$)

(b) Potential elevations on cross sections
Fig. 4 Potential after one rotation
(by 3rd-order upwind difference method : $\alpha=1$)

(a) Potential contours
(red : $\phi=0.01$, yellow : $\phi=0.5$)

(b) Potential elevations on cross sections
Fig. 5 Potential after one rotation
(by QUICKEST method)

methods are almost the same. Though the QUICK method is a 2nd-order spatial discretization method, the damping of potential is smaller than those of the 3rd-order spatial discretization methods, and error E of this method is close to those of the 3rd-order spatial discretization methods. The $\phi_{\max}$ and E of the 4th-order centered difference method are not affected by θ . The damping of the potential by this method is slight, but the spurious spatial oscillation can be observed at the upwind of the potential sphere in Figs. 6(a) and 6(b). With the 5th-order upwind method, the damping of the potential is slight and the spatial oscillation is not produced. Thus the root mean square error is considerably improved. The sixth-order differential term, the major truncation error of the 5th-order upwind method, is especially effective for the damping of high-wave-number spatial oscillation.

With the 6th-order centered difference method, the damping and the root mean square error are fairly good, but slight spurious spatial oscillation is produced at the upwind of the potential sphere in Figs. 8(a) and 8(b).

The larger θ becomes, the larger the damping of the potential becomes when the upwind difference methods are applied. With the application of the centered difference methods, the damping of the potential is not affected by θ .

The larger θ becomes, the larger the root mean square error becomes except when the 4th-order centered difference method is applied, but the differences in the root mean square error are slight.

The numerical results are not affected by the time step Δt when it is in the range in which computations are stable. The 2nd-order Adams-Bashforth method is also applied as a time integration method. There is

(a) Potential contours
(red : $\phi=0.01$, yellow : $\phi=0.5$)

(b) Potential elevations on cross sections

Fig. 6 Potential after one rotation
(by 4th-order centered difference method)

(a) Potential contours
(red : $\phi=0.01$, yellow : $\phi=0.5$)

(b) Potential elevations on cross sections

Fig. 7 Potential after one rotation
(by 5th-order upwind difference method : $\alpha=1$)

no great difference between the results of the 2nd-order Adams-Bashforth and those of the 3rd-order Adams-Bashforth when the upwind difference methods are applied as spatial discretization methods. When the 2nd-order Adams-Bashforth and the centered difference methods are applied simultaneously, computations are unstable.

Figure 10 shows the root mean square error for mesh width $\Delta x = 1/25, 1/20, 1/15$ and $1/10$, i.e., 125 000, 64 000, 27 000 and 8 000 uniform mesh, respectively. The Courant number at the center of potential sphere is 0.15, $\theta = 45^\circ$, and the 3rd-order Adams-Bashforth method is applied for the time integration method. The finer the mesh applied, the smaller the root mean square error becomes. The root mean square error of the QUICK method, the 3rd-order upwind difference method and the QUICKEST method increases faster than the error of the 2nd-order centered difference method with increase of mesh width. Moreover the

error of the 4th-order centered method, the 5th-order upwind method and the 6th-order centered method increases faster than the error of the QUICK method, the 3rd-order upwind difference method and the QUICKEST method with increase of mesh width. Therefore the higher-order spatial discretization method does not always provide a more accurate solution.

5. Conclusions

Some typical finite difference methods have been evaluated by computing the three-dimensional advection equation, i.e., the rotating sphere problem, and we can conclude as follows.

(a) Potential contours
(red : $\phi = 0.01$, yellow : $\phi = 0.5$)

(b) Potential elevations on cross sections

Fig. 8 Potential after one rotation
(by 6th-order centered difference method)

Fig. 9 Root mean square error against θ

Fig. 10 Root mean square error against mesh width

(1) When the 2nd-order Adams-Bashforth or 3rd-order Adams-Bashforth is applied to the three-dimensional advection equation, the results are not affected by the time step Δt only if it is the range of Courant numbers which provides a stable solution.

(2) When fine mesh with a mesh number of 27 000 or over is used, the higher-order the spatial discretization becomes, the smaller the root mean square error becomes. But when the mesh is coarse, with a mesh number of 8 000 or under, the higher-order spatial discretization method does not always provide a more accurate solution.

(3) By applying a higher-order spatial discretization method, we can reduce the mesh number considerably without losing accuracy. For example, the solution obtained by the 5th-order upwind difference method with 27 000 mesh is more accurate than that obtained by the 3rd-order upwind difference method with 125 000 mesh.

(4) When upwind difference methods are applied, the larger θ , the angle formed by the z -axis and the rotating axis, becomes, the larger the damping of the

potential becomes. This means that the larger θ becomes, the larger the artificial viscosity becomes.

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