RESEARCH PAPERS

Compact difference approximation with consistent boundary condition*

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Abstract For simulating multi-scale complex flow fields it should be noted that all the physical quantities we are interested in must be simulated well. With limitation of the computer resources it is preferred to use high order accurate difference schemes. Because of their high accuracy and small stencil of grid points computational fluid dynamics (CFD) workers pay more attention to compact schemes recently. For simulating the complex flow fields the treatment of boundary conditions at the far field boundary points and near far field boundary points is very important. According to authors' experience and published results some aspects of boundary condition treatment for far field boundary are presented, and the emphasis is on treatment of boundary conditions for the upwind compact schemes. The consistent treatment of boundary conditions at the near boundary points is also discussed. At the end of the paper are given some numerical examples. The computed results with presented method are satisfactory.

Keywords: complex flow fields, numerical simulation, boundary conditions, upwind compact scheme.

For correct simulation of unsteady complex flow fields with multi-scale structures it is required that all the physical scales we are interested in must be captured well. There are two ways to improve the resolution. One is to refine the mesh grid system, and the other is to use high order accurate schemes. Because of limitation of computer resources it is preferred to use high order accurate schemes to solve the complex flow fields like turbulence. Many good high order schemes have been developed. Because of high accuracy and small stencil CFD scientists pay more attention to the compact difference schemes[1~4]. Within the compact schemes the upwind compact schemes have smaller aliasing errors.

With given method the treatment of boundary conditions is a key problem for correct simulation. It influences the accuracy of solutions and the stability of method.

In numerical simulation of complex flow fields there are two kinds of boundary conditions. One of them is the physical conditions. For discretization of this kind of condition attention should be paid to accuracy of discretization and stability. The other kind of boundary condition is not required by physics. They are additional due to discretization of the partial differential equations. For the high order accurate schemes larger stencil of grid points requires more additional conditions not only at the boundary but also at the near boundary points.

As it is noted, for simulating the complex flow field like turbulence it is preferred to use the high order schemes. For the typical turbulent problems the computational domain is limited. Before simulating the chosen physical problems we have to define the computational domain. The computational domain should be defined so that treatment of the boundary conditions does not disturb the flow structures we are interested in. With chosen method and properly defined computational domain the success of simulation directly depends on the treatment of the boundary conditions at the boundaries and at the near boundary points especially for the compact schemes. It is required that the disturbance from the outside or produced at the boundaries and near boundary points should not be propagated into the interior domain of the computation. The boundary conditions treated in this way are considered as the non-reflected boundary

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conditions.

People start to study the boundary conditions from the middle of the last century. Kriess obtained a sufficient condition of stability for a two-level explicit scheme for the initial-boundary problem[1)]. In [5] Gustafsson, et al. obtained a sufficient condition of stability for multi-level implicit scheme, and their result is called GKS theory. In [4] Lele discussed boundary conditions for the compact schemes, and Poinsot and Lele in [6] presented non-reflection boundary condition for solving the complex flow fields. According to the upwind compact finite difference schemes authors of this paper give a much simpler non-reflection boundary condition. When the non-reflection treatment is introduced usually the approximation at the near boundary points is not consistent for the compact difference approximation. Consistent boundary conditions for the third and fifth order accurate upwind compact difference approximation at the near boundary points are presented in this paper.

Usually people use the high order accurate symmetrical difference approximation to simulate the complex multi-scale flow fields. Their thought is that the upwind schemes are too dissipative, and some fine flow structures may be smeared out. Our experience shows that the high order accurate upwind schemes can also give good resolution for the complex flow fields. In the present paper we first give a numerical example to show the efficiency of upwind compact schemes for simulating the complex flow structures, and then present far field non-reflection boundary conditions for simulating the complex flows and the consistent treatment at the near boundary points for the third and fifth order accurate upwind compact difference approximations. In the end of this paper some numerical experiments are presented.

1 Aliasing error and dissipative scheme

When functions are represented in terms of a finite number of basis functions, nonlinear operations generate modes that are not in the set of modes being represented. A discrete representation mistakes these high order modes for modes in the set. There are two kinds of errors after the nonlinear operations. One of them is that the effect of some high order modes are not taken into account. This part of errors is called nonlinear truncation errors. The other one is that the contribution from these high order modes is improperly added to the modes in the set. The second is called aliasing errors.

There are two ways to overcome the errors produced in the nonlinear operations. One of them is to refine the mesh grid system, but it is limited by computer resources. The other one is to construct high order accurate schemes, for example, the compact difference schemes. For the symmetrical schemes there are mainly dispersion errors. For the upwind schemes there are dispersive and dissipative errors. From analysis of modified wave numbers we can see that in wide range of wave numbers the dispersion errors for both the symmetrical and upwind schemes with the same order of accuracy of approximation are almost the same. From linear analysis we can also see that the dissipativity of the upwind compact schemes in the range of wave numbers for correct representation of dispersion effect is negligible. The dissipation is large only for the components with high wave numbers. The large dissipativity for high wave numbers is useful for reduction of the aliasing errors.

The numerical experiment in Ref. [7] shows that with the same mesh grid system the fifth order accurate upwind compact scheme has smaller aliasing errors than the spectral method does. In Ref. [8] the fifth order accurate upwind compact difference approximation is used to simulate the homogeneous isotropic turbulence. The variation of turbulent kinetic energy with initial turbulent Mach number $Mt(t=0)=0.5$ is given in Fig. 1. The computed results with upwind compact scheme (UCFD5) agree well with the results with the tenth order Pade scheme with the same mesh grid system in Ref. [9]. From the computed results we can also see that the fifth order WENO scheme is too dissipative.

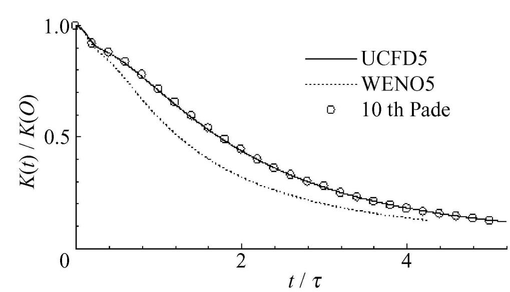

Fig. 1. Variation of normalized turbulent kinetic energy ($Re_\lambda = 72$, $Mt(0)=0.5$).

1) Kriess, O.H. AGARD-LS-64, 1973.

This numerical example shows that the high order accurate upwind compact schemes can be used to simulate the multi-scale complex flow fields like turbulence. Because of limitation of computer resources recently the direct numerical simulation (DNS) can be used only for the flows with low Reynolds number to study the mechanism of turbulence.

2 Non-reflection and consistent boundary conditions

From analysis and numerical experiment we know that the high order accurate compact schemes are a kind that can be chosen to correctly simulate the multi-scale complex flow fields. For DNS first we have to define the computational domain and the boundaries of computation. The boundaries should be defined so that the targeted flow structures in the subdomain should not be affected by the disturbance produced at the boundaries, that is, the correlation of the flow parameters between the boundary points and the points in the subdomain in which the flow structures we are interested in should be small.

There are two kinds of boundaries of computation. One is the physical boundary like the wall of channel flow. The physical boundary conditions should be given at the wall boundary. The other kind is like the downstream boundary for the flow around the flat plat or the boundary far from the wall which is defined by CFD workers. The physically properly chosen boundaries do not provide small influence of boundary condition treatment. At this kind of boundary the physical parameters cannot be defined before computation. Treatment of this kind of boundary condition should be stable and does not affect the inner flow structures much. Practice shows that so called non-reflection boundary treatment can usually give good results. In this paper we consider how to define the conditions at this kind of far field boundary.

For simplicity consider the following Euler equations

$$\frac{\partial \boldsymbol{U}}{\partial t} + \frac{\partial \boldsymbol{f}}{\partial x} = 0, \qquad (1)$$

where $\boldsymbol{U}$ is the vector of conservative variables, $\boldsymbol{f}$ the flux vector. The simplest fourth order accurate symmetrical compact difference approximation is

$$\frac{1}{6}\boldsymbol{F}_{j+1} + \frac{2}{3}\boldsymbol{F}_j + \frac{1}{6}\boldsymbol{F}_{j-1} = \delta_x^0 \boldsymbol{f}_j, \qquad (2)$$

where

$$\delta_x^0 \boldsymbol{f}_j = \frac{1}{2}(\delta_x^+ + \delta_x^-)\boldsymbol{f}_j, \quad \delta_x^\pm \boldsymbol{f}_j = \mp(\boldsymbol{f}_j - \boldsymbol{f}_{j\pm1}),$$

$$\boldsymbol{F}_j / \Delta \boldsymbol{x} \approx \left(\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}\right)_j.$$

Usually the gradient of the fluid parameters at far field boundaries is small and it can be assumed to be equal to zero. For example, $\boldsymbol{F}_j(\boldsymbol{j} = \boldsymbol{JN}) = 0$. In this case Eq. (2) turns into

$$\frac{2}{3}\boldsymbol{F}_{JN-1} + \frac{1}{6}\boldsymbol{F}_{JN-2} = \delta_x^0 \boldsymbol{f}_{JN-1}. \qquad (3)$$

After Taylor series expansion we can see that $\boldsymbol{F}_j / \Delta x \approx \frac{6}{5}\frac{\partial \boldsymbol{f}}{\partial x}$. It means that the difference expression (3) is not consistent. It is assumed that the gradient of fluid parameters is small at the boundary. From the point of view of accuracy the inconsistency does not influence much the accuracy of solution. But inconsistency of approximation may lead to the change of the property of the equations or lead to instability of solutions. It is suggested to use consistent difference approximation.

For construction of upwind schemes after flux splitting Eq. (1) can be rewritten as

$$\frac{\partial \boldsymbol{U}}{\partial t} + \frac{\partial \boldsymbol{f}^+}{\partial x} + \frac{\partial \boldsymbol{f}^-}{\partial x} = 0, \qquad (4)$$

where the term with $\boldsymbol{f}^+$ describes the motion of fluid components from the left to the right, and the term with $\boldsymbol{f}^-$ describes the motion from the right to the left.

The third order accurate upwind compact difference approximation of the convection terms in Eq. (4) is expressed as

$$\frac{2}{3}\boldsymbol{F}_j^\pm + \frac{1}{3}\boldsymbol{F}_{j\mp1}^\pm = \left(\frac{5}{6}\delta_x^\mp + \frac{1}{6}\delta_x^\pm\right)\boldsymbol{f}_j^\pm, \qquad (5)$$

where $\boldsymbol{F}_j^\pm / \Delta \boldsymbol{x} \approx (\partial \boldsymbol{f}^\pm / \partial \boldsymbol{x})_j$. In Ref. [6] it is required that the disturbance on the boundary does not propagate into the computational domain. Their governing equations are transformed into the characteristic form. The terms in the characteristic equations describing the movement from inner points into outside of the computational domain are discretized by the first order accurate difference approximation, and the terms describing the movement from outside into the computational domain are set to zero. When the upwind schemes are used the non-reflection boundary conditions can be treated easily. We can simply let the term $\partial \boldsymbol{f}^- / \partial \boldsymbol{x}$ equal zero in Eq. (4) at the boundary $J = JN$, and the upwind difference approximations can be used to discretize the term $\partial \boldsymbol{f}^+ / \partial \boldsymbol{x}$.

With this assumption we have

$$F_{JN}^{-} = 0. \tag{6}$$

Now we have got a simple non-reflection boundary condition at the boundary $J = JN$.

With this assumption the difference relation (5) for the split flux f_j^- at the point $JN-1$ has the form

$$\frac{2}{3}F_{JN-1}^{-} = \left(\frac{5}{6}\delta_x^+ + \frac{1}{6}\delta_x^-\right)f_{JN-1}^{-}. \tag{7}$$

It is obvious that relation (7) is an inconsistent difference approximation for f_j^-. A consistent difference approximation is

$$F_{JN-1}^{-} = \delta_x^+ f_{JN-1}^{-}. \tag{8}$$

This treatment is consistent, and the characteristic direction is taken into account. Like in Ref. [6] the approximation is the first order. As it has been noted that the gradient of fluid parameters is assumed to be small near the far field boundary, the accuracy of approximation is accepted.

The difference approximation (5) for the component f_j^+ at the point $j = JN-1$ is normal and no special treatment is needed. The following simple difference approximation can be used for the component f^+ at the point $j = JN$,

$$F_{JN}^{+} = \frac{1}{2}(3\delta_x^- f_{JN}^{+} - \delta_x^- f_{JN-1}^{+}). \tag{9}$$

This treatment is consistent, and the characteristic direction is taken into account.

In the same way we can construct the non-reflection boundary conditions and the consistent difference approximations at and near the left boundary.

We can also easily construct non-reflection boundary conditions and the consistent difference approximation at and near the boundary points for the fifth order accurate upwind compact difference scheme. For the left going component relation (6) can also be used as the non-reflection condition at the point $j = JN$, but the point $j = JN-1$ is not the normal point for the fifth order upwind compact difference approximation. In this case we have to use approximation (8) or construct the higher order consistent approximation by the following expression

$$\alpha F_{JN-1}^{-} + \beta F_{JN}^{-} = \delta_x^+(af_{JN-1}^{-} + bf_{JN-2}^{-} + cf_{JN}^{-}), \tag{10}$$

where the free parameters need to be defined. From (10) we can construct the fifth order approximation, but in order that the approximation is consistent we have to reduce the order of approximation by adjusting the parameters. Considering (6) together with $\delta_x^+ f_{JN}^- = 0$, after Taylor series expansion the following consistent difference approximation at the point $j = JN-1$ can be obtained:

$$\frac{4}{3}F_{JN-1}^{-} = \delta_x^+\left(\frac{5}{6}f_{JN-1}^{-} + \frac{1}{2}f_{JN-2}^{-}\right). \tag{11}$$

The third order accurate upwind compact difference approximation at the point $j = JN-1$ and the approximation (9) at the point $j = JN$ for the component f^+ can be used for the fifth order upwind scheme.

3 Numerical experiment

The above presented method for construction of the non-reflection boundary difference approximation at the far field boundaries and the consistent difference approximations at the near boundary points are used to simulate one-dimensional, two-dimensional and three-dimensional practical problems. Only some 2-D and 3-D results are presented here.

3.1 Two-dimensional vortex propagation

The two-dimensional compressible Navier-Stokes (N-S) equations are used to simulate the vortex propagation. The purpose is to see the efficiency of presented method for treatment of difference approximation at the boundary and near boundary points. The convection terms of the N-S equations are discretized with the fourth order accurate upwind compact difference approximation, and the viscous terms are discretized with the symmetrical fourth order accurate compact approximation, and the three stage TVD R-K method is used in advance of time.

The fluid parameters in computation are $Ma = 1.2$, $Re = 2000$. The initial distribution of the fluid parameters consists of a uniform field plus a perturbation. The uniform field is

$$u = 1,\quad v = 0,\quad T = 1,\quad \rho = 1 \tag{12}$$

and the perturbations for the velocity components are

$$\begin{aligned} u_\theta'(r) &= M_v \exp[(1 - r^2)/2], \\ u_r' &= 0, \end{aligned} \tag{13}$$

where r is the radius $r = (x^2 + y^2)^{1/2}$, u_θ the tangential velocity component, u_r the radial velocity component, and M_v the rotation Mach number. In computation $M_v = 0.5$ is used. The density perturbation is taken as

$$\rho'(r) = \left[1 - \frac{\gamma - 1}{2} M_v^2 \exp(1 - r^2)\right]^{\frac{\gamma}{\gamma - 1}} - 1. \tag{14}$$

The vortex contours at $t=0$ are given in Fig. 2, and the vortex contours at $t=4.0$ are given in Fig. 3. From Fig. 3 we cannot see the upstream propagating waves after interaction of the vortex with the boundary.

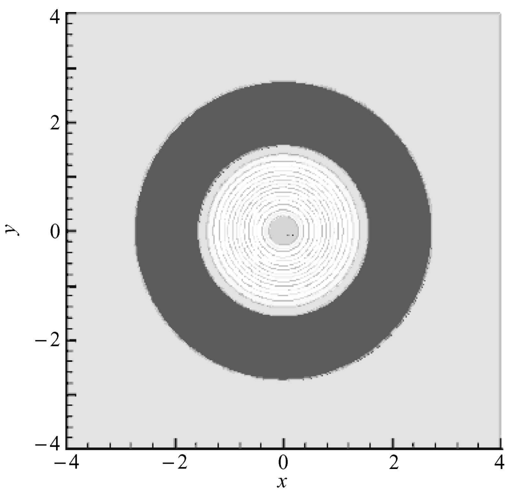

Fig. 2. Vortex contours at $t=0.0$.

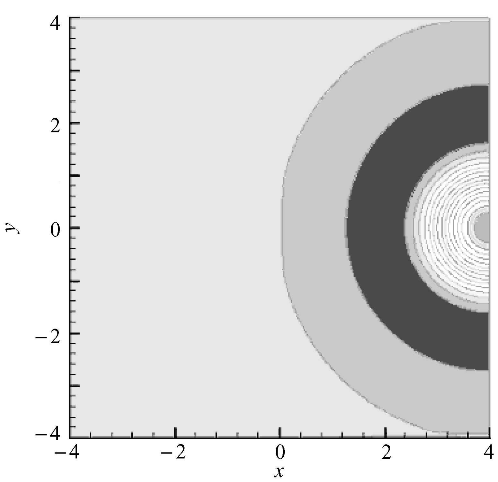

Fig. 3. Vortex contours at $t=4.0$.

The non-consistent difference approximation (7) is also used to compute the same problem, and it is found that the result is also acceptable. This is because the difference approximation is dissipative. The same problem is also computed with condition (6) with zero gradient of physical parameters, but the computation is unstable.

3.2 Simulation of the three-dimensional compressible jet

The three-dimensional N-S equations are used to simulate a three-dimensional round jet with incoming Mach number $Ma = 0.2, 0.6, 0.9$ and Reynolds number $Re = 15000$ based on the inlet diameter and incoming flow velocity. The convection terms of the N-S equations are discretized with the 5th order accurate upwind compact difference approximation, the viscous terms are discretized with the 6th order accurate symmetrical compact difference approximation, and a TVD R-K method is used in advance with time. At the side boundaries and downstream boundary the above presented treatment is used. The computed results are satisfactory.

The complete process of flow structure development can be obtained from K-H instability, production of azimuthal vortices, the second instability and formation of the streamwise vortices to turbulent transition. The contours of the passive function on meridian plan $(0,\pi)$ for the case $Ma=0.2$ are given in Fig. 4 from which we can see the process of flow structure development. The variation of the momentum thickness in the streamwise direction is given in Fig. 5 from which we can see the sudden change near the point $x \approx 3$ where the second instability starts and $x \approx 10$ where the flow translation starts. By using the data of direct numerical simulation the effect of compressibility on formation and development of three-dimensional coherent structures is discussed in details.

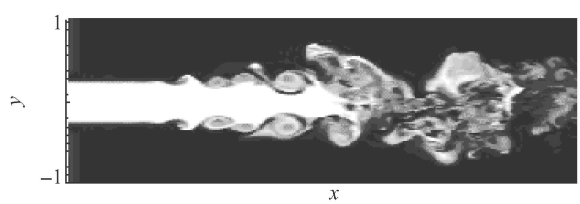

Fig. 4. Distribution of scale function on meridian $(0,\pi)$.

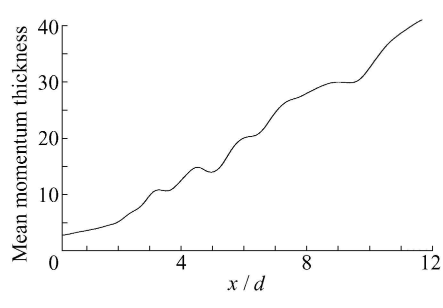

Fig. 5. Variation of momentum thickness with x/d ($Ma=0.2$, d-diameter).

4 Summary

Recent progress of the far field non-reflecting boundary conditions is presented briefly. The emphasis of this paper is on development of new simpler non-reflecting far field boundary conditions for upwind compact difference approximations. It is suggested to use consistent difference approximation at the near boundary points. Numerical experiments show that the computed results are satisfactory with the presented boundary condition treatment.

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