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A modified finite volume method for convection-diffusion-reaction problems

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ABSTRACT

Usually for the conventional numerical methods the increase of their accuracy and stability is at the cost of increasing the size of the computational stencil. In the present work, without widening the computational stencil of the classical finite volume method (FVM) we propose a modified finite volume method (MFVM) which is much more accurate and stable than the FVM. In the MFVM some undetermined coefficients are introduced in discretizing the convection-diffusion-reaction equation. These coefficients are determined analytically by making the truncation error of the numerical scheme vanish and by expressing the high order derivatives of the unknown function with low order ones through the governing equation. Interestingly, for some one-dimensional convection-diffusion-reaction problems the MFVM can achieve almost the same accuracy as the exact solution, and does not induce any unphysical oscillations for the convection/reaction-dominated problems.

1. Introduction

Convection-diffusion-reaction processes are involved in many important engineering systems, such as nuclear reactors, chemical reaction processes and environmental pollution treatment. Its governing equation reads:

$$\frac{\partial(\rho u\phi)}{\partial x}+\frac{\partial(\rho v\phi)}{\partial y}+\frac{\partial(\rho w\phi)}{\partial z}+r\phi = \frac{\partial}{\partial x}\left(\Gamma\frac{\partial\phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(\Gamma\frac{\partial\phi}{\partial y}\right)+\frac{\partial}{\partial z}\left(\Gamma\frac{\partial\phi}{\partial z}\right)+f(x,y,z) \quad (1)$$

where $(x,y,z)^T \in D$ is the position vector and D is the fluid domain, ρ is the fluid density, $(u,v,w)^T$ is a given velocity field, ϕ is a conserved property, f is the source term, r and Γ are reaction and diffusion coefficients, respectively. There are two important parameters charactering the convection-diffusion-reaction processes. One is the Peclet number which is defined as $Pe=\rho UL/\Gamma$ (here U is the characteristic velocity, L is the characteristic length); another is the Damkohler number Da defined as $Da=rL/U$. It is a notorious problem to numerically solve the convection/reaction-dominated transport phenomena with the high Pe and Da which induces thin boundary or interior layers. In these layers the field variables vary steeply, which leads to a low accuracy and lack of stability for the convectional numerical methods. To overcome this difficulty, several stabilizing schemes have been proposed.

In the framework of the finite element method (FEM), some stabilized finite element methods have been designed [1–6]. In the finite difference method (FDM) and FVM, the basic upwind differencing scheme (UDS) is the most stable and unconditionally bounded scheme. However, its low order of accuracy introduces a high level of false diffusion. Although the upwind compact difference schemes have improved the accuracy of the UDS significantly [7–10], they usually need large size stencils in comparison with the UDS. In order to avoid the unphysical oscillations near discontinuities, the Total Variation Diminishing (TVD) scheme has been developed [11]. The TVD solutions of convection-diffusion problems show far less false diffusion than UDS. Moreover, they do not introduce any unphysical overshoots and undershoots. However, all TVD schemes will degenerate to lower order accuracy near local smooth extrema [12]. In addition, the TVD scheme would consume more CPU-time than the traditional UDS [13]. Based on a different approach, Harten et al. (1987) proposed a self-similar, uniformly high accurate, and essentially non-oscillatory (ENO) interpolation for piecewise smooth function in solving hyperbolic partial differential equations [14]. Later, the weighted ENO (WENO) schemes were developed by using a convex combination of all candidate stencils instead of just one as in the original ENO [15]. The WENO reconstructions are very successful in capturing shocks in a non-oscillatory fashion while maintaining high accuracy in smooth regions. However, Shen and Zha found that the

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fifth-order WENO scheme will degenerate to the third order at a transition point near discontinuities [16]. In addition, the WENO schemes require uniform or at lease smoothly varying mesh size [17]. Furthermore, the WENO schemes are not favorable to simulate the small scale turbulent flows [18].

Because of the simplicity and conservation of the physical laws, the FVM is widely applied in simulating the fluid dynamic and heat transfer problems. The control volume integration is the key step in the FVM which maintains the conservation of the relevant properties for each finite size cell. Actually, the control volume integration can reduce the order of the highest derivative that appears in the governing equations of fluid flows and heat transfers, which weakens the requirement of the smoothness of the unknown function. According to this methodology some integration methods for the convection-diffusion-reaction problems have been developed. An axial Green's function method (AGM) was proposed for solving the multi-dimensional elliptic boundary value problems [19]. Later, it was extended to simulate the Stokes flow [20]. A local axial Green's function method which is the localization of the AGM was established for solving the convection-diffusion equation [21]. Similarly, a nonstandard finite difference scheme based on the Green's function formulation was proposed for solving the convection-diffusion-reaction problems [22]. Recently, a finite integration method was proposed for solving partial differential equations by using numerical quadrature or radial basis function interpolation [23]. Based on the Green's function in a series form and the integration formulation, an integral equation approach was established for simulating the steady hydromagnetic dynamo [24], the magnetic reconnection phenomena [25] and the convection-diffusion problems [26,27].

As pointed out by Skála et al., usually the high order schemes are numerically expensive [28]. For example, Nth-order classical FDM requires a stencil including *N+1* grid points. The increase of the stencil size not only means more requirements of the CPU memory, but also more computing work. Although the compact FDM can reduce the stencil size and increase the accuracy of the FDM, the high order compact FDM still need large size of computational stencil in comparison with the low order compact FDM [29,30]. Therefore, it is still of great importance to design numerical methods which has a same size stencil as that of the traditional FVM on the one hand, and accurate and robust on the other hand for simulating the complicated phenomena of fluid dynamics and manetohydrodynamics, such as turbulence, magnetic reconnection and dynamo actions. Recently, we have proposed a series of high order schemes for solving the convection-diffusion problems by integrating the convection-diffusion equation expressed as the first order partial differential equations over selected regions and applying the numerical quadrature with a weighting parameter for approximating the resulting integrals [31]. Interestingly, the weighting parameter in the numerical quadrature can be determined analytically by making the error of the numerical scheme as small as possible. In the present work, we attempt to extend this methodology to improve the traditional FVM for solving the convection-diffusion-reaction problems. Our goal is to slightly modify the traditional FVM, but to significantly improve its stability and accuracy for dealing with the convection/reaction-dominated transport phenomena.

2. Discretization algorithm

Consider the three-dimensional convection-diffusion-reaction equation (1). Define the transport fluxes J_x, J_y and J_z in the x-, y- and z-direction are as follows

$$J_x = \rho u\phi - \Gamma\frac{\partial\phi}{\partial x},\quad J_y = \rho v\phi - \Gamma\frac{\partial\phi}{\partial y},\quad J_z = \rho w\phi - \Gamma\frac{\partial\phi}{\partial z} \tag{2}$$

Substituting Eq. (2) into (1) yields

$$\frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z} + r\phi = f \tag{3}$$

Next the grid points $(x_i,y_j,z_k)^T$ $(i=0,1,2,\cdots,M;j=0,1,2,\cdots,N;k=0,1,2,\cdots,K)$ are employed to divide the fluid domain D. The volume $[x_{i+1/2},x_{i+3/2}]\times[y_{j+1/2},y_{j+3/2}]\times[z_{k+1/2},z_{k+3/2}]$ with $x_{i+1/2}=x_i+0.5(x_{i+1}-x_i)$ and $x_{i+3/2}=x_{i+1}+0.5(x_{i+2}-x_{i+1})$ is taken as the control volume around the node point $(x_{i+1},y_{j+1},z_{k+1})^T$. Integrating Eq. (3) over the control volume yields

$$\begin{aligned}&\left(J_{x,i+3/2,j+1,k+1}-J_{x,i+1/2,j+1,k+1}\right)\left(y_{j+3/2}-y_{j+1/2}\right)\left(z_{k+3/2}-z_{k+1/2}\right)\\&+\left(J_{y,i+1,j+3/2,k+1}-J_{y,i+1,j+1/2,k+1}\right)\left(x_{i+3/2}-x_{i+1/2}\right)\left(z_{k+3/2}-z_{k+1/2}\right)\\&+\left(J_{z,i+1,j+1,k+3/2}-J_{z,i+1,j+1,k+1/2}\right)\left(x_{i+3/2}-x_{i+1/2}\right)\left(y_{j+3/2}-y_{j+1/2}\right)\\&+(r\phi)_{i+1,j+1,k+1}(\beta_x+\beta_y+\beta_z)(x_{i+3/2}-x_{i+1/2})(y_{j+3/2}-y_{j+1/2})\\&\times(z_{k+3/2}-z_{k+1/2})/3=f_{i+1,j+1,k+1}(x_{i+3/2}-x_{i+1/2})(y_{j+3/2}-y_{j+1/2})\\&\times(z_{k+3/2}-z_{k+1/2})\end{aligned} \tag{4}$$

with

$$\begin{aligned}f_{i+1,j+1,k+1}=&\int_{x_{i+1/2}}^{x_{i+3/2}}\int_{y_{j+1/2}}^{y_{j+3/2}}\\&\times\int_{z_{k+1/2}}^{z_{k+3/2}}f dz dy dx\Big/\Big[(x_{i+3/2}-x_{i+1/2})(y_{j+3/2}-y_{j+1/2})\\&\times(z_{k+3/2}-z_{k+1/2})\Big]\end{aligned}$$

Eq. (4) is rewritten as follows:

$$\begin{aligned}&\left(J_{x,i+3/2,j+1,k+1}-J_{x,i+1/2,j+1,k+1}\right)/(x_{i+3/2}-x_{i+1/2})\\&+\left(J_{y,i+1,j+3/2,k+1}-J_{y,i+1,j+1/2,k+1}\right)/(y_{j+3/2}-y_{j+1/2})\\&+\left(J_{z,i+1,j+1,k+3/2}-J_{z,i+1,j+1,k+1/2}\right)/(z_{k+3/2}-z_{k+1/2})\\&+(r\phi)_{i+1,j+1,k+1}(\beta_x+\beta_y+\beta_z)/3=f_{i+1,j+1,k+1}\end{aligned} \tag{5}$$

where β_x, β_y and β_z are undetermined coefficients which will be determined by the error analysis. The values of the fluxes at the cell faces are evaluated in the following way:

$$\begin{aligned}J_{x,i+1/2,j+1,k+1}&=(\rho u\phi)_{i+1/2,j+1,k+1}-\left(\Gamma\frac{\partial\phi}{\partial x}\right)_{i+1/2,j+1,k+1}\\&=\left[\alpha_{1x}(\rho u\phi)_{i+1,j+1,k+1}+(1-\alpha_{1x})(\rho u\phi)_{i,j+1,k+1}\right]\\&\quad-\Gamma_{i+1/2,j+1,k+1}(\phi_{i+1,j+1,k+1}-\phi_{i,j+1,k+1})/(x_{i+1}-x_i)\end{aligned} \tag{6}$$

Note that in Eq. (6) the value of the flux at the cell face is evaluated by taking the weighted arithmetic mean of the values of the two neighbor node points. The weight α_{1x} will be determined by letting the truncation error vanish. For the traditional central difference scheme (CDS) the weight is just taken as 0.5, that is, the contribution of the neighbor downstream and upstream node points to the flux at the cell face is equal. Thus the traditional CDS has not reflected the flow direction, which is the main reason that the CDS is unstable when the Peclet number is large. In analogous with Eq. (6) we have

$$\begin{aligned}J_{x,i+3/2,j+1,k+1}&=(\rho u\phi)_{i+3/2,j+1,k+1}-\left(\Gamma\frac{\partial\phi}{\partial x}\right)_{i+3/2,j+1,k+1}\\&=\left[\alpha_{2x}(\rho u\phi)_{i+2,j+1,k+1}+(1-\alpha_{2x})(\rho u\phi)_{i+1,j+1,k+1}\right]\\&\quad-\Gamma_{i+3/2,j+1,k+1}(\phi_{i+2,j+1,k+1}-\phi_{i+1,j+1,k+1})/(x_{i+2}-x_{i+1})\end{aligned} \tag{7}$$