NOTE

A Slope-Update Scheme for Compressible Flow Simulation

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Received November 3, 2000; revised February 22, 2002

Key Words: MUSCL-type scheme; Euler equations; gas-kinetic scheme; slope-update method.

1. INTRODUCTION

The traditional MUSCL-type schemes consist of three stages [7], the initial reconstruction, the gas evolution, and the projection. In the reconstruction stage, a nonlinear limiter based on TVD or ENO concepts is used for the initial subcell data reconstruction at the beginning of each time step. In order to get a high spatial resolution, a stencil involving a large number of grid points is needed. In the gas-evolution stage, based on the reconstructed initial data, the fluid-dynamic equations are solved to evaluate a numerical flux across each cell interface, from which the conservative variables inside each cell are updated in the projection stage. In many flow applications with unstructured mesh, the appropriate reconstruction of the initial data inside each element requires a great amount of CPU time and computer memory. The objective of this note is to point out that if a time-accurate solution can be obtained in the gas-evolution stage, not only the conservative variables but also their slopes can be updated in a numerical scheme. Therefore, even with the stencil of a first-order scheme, a high-resolution method can be constructed. The idea of slope update is not new in the literature. For example, the discontinuous Galerkin (DG) method and Hermitian methods use that. van Leer also stressed the idea of retaining not only cell averages but slopes as well [7]. Recently, the slope update was successfully implemented in the central

1 Research was supported by Hong Kong Research Grant Council through DAG 01/02.SC19.
difference CE/SE method [3]. Similar to the scheme by Nessyahu and Tadmor [5], the success of central schemes, such as the robustness and high accuracy, depends much on the use of a staggered mesh. In this note, a slope-update method is constructed for the gas-kinetic BGK scheme, where a nonstaggered mesh is used. In our approach, the time-dependent flow variables at a cell interface, which are used for the local slope construction in the next time step, are explicitly evaluated. This approach is different from solving the slope-governing equation in the DG method. A few numerical examples are included to validate the current approach.

2. SLOPE-UPDATE METHOD

For the compressible flow simulations, the gas-kinetic BGK scheme has been successfully developed and applied to many physical and engineering problems [9]. Similar to many finite-volume schemes, the gas-kinetic method is based on a MUSCL-type approach, where a nonlinear limiter is used for the initial data reconstruction, and the gas-kinetic equation is solved to evaluate a time-dependent gas distribution function at a cell interface, from which the numerical fluxes are obtained (see Fig. 1). Due to the intrinsic connection between the gas-kinetic BGK model and the Navier–Stokes equations, a Navier–Stokes solution is obtained automatically from the BGK scheme without splitting the inviscid and viscous terms [10]. Currently, many flow solvers are based on the gas-kinetic BGK model, such as the lattice Boltzmann method (LBM) [4] and discrete velocity model (DVM) [2]. The merit of the current approach is the explicit coupling of the particle transport and collision. Most other methods decouple the transport and collision, and the decoupling automatically introduces an intrinsic numerical dissipation which is proportional to the time step [10]. Therefore, if the numerical dissipation due to the decoupling cannot be interpreted properly as a “physical” one, it is required that the particle collision time be much larger than the time step in order to have the physical dissipation become dominant such as in the Direct Simulation Monte Carlo (DSMC) method.

For the 1D flow, the BGK model in the $x$-direction is [1]

$$f_i + u f_i' = \frac{g - f}{\tau},$$

(1)

where $f$ is the gas distribution function and $g$ is the equilibrium state approached by $f$.

**FIG. 1.** Mass $\rho$, momentum $\rho U$, and energy $\rho E$ distributions, which are used as initial conditions for evaluating a time-dependent gas distribution function at the cell interface $x_{j+1/2}$ in the gas-kinetic BGK scheme.
The particle collision time $\tau$ is related to the viscosity and heat conduction coefficients. The equilibrium state is a Maxwellian distribution, 

$$g = \rho \left( \frac{\lambda}{\pi} \right)^{\frac{3}{2}} e^{-\lambda((u-U)^2+\xi^2)}$$

where $\rho$ is the density, $U$ is the macroscopic velocity in the $x$-direction, and $\lambda$ is related to the gas temperature $m/2kT$. The total number of degrees of freedom $K$ of $\xi$ is equal to $(5 - 3y)/(y - 1)$. In the equilibrium state, $\xi^2$ is equal to $\xi_1^2 + \xi_2^2 + \cdots + \xi_K^2$. The relation between mass $\rho$, momentum $\rho U$, and energy $\rho E$ densities with the distribution function $f$ and the equilibrium state is 

$$w = (\rho, \rho U, \rho E)^T = \int \psi_\alpha f \, d\Xi = \int \psi_\alpha g \, d\Xi, \quad \alpha = 1, 2, 3,$$

where $\psi$ is the vector with components 

$$\psi = \left( 1, u, \frac{1}{2} (u^2 + \xi^2) \right)^T,$$

and $d\Xi = du \, d\xi$ is the volume element in the phase space with $d\xi = d\xi_1 \, d\xi_2 \ldots d\xi_K$.

The BGK scheme is based on the integral solution $f$ of the BGK model at a cell interface $x_{j+1/2}$, 

$$f(x_{j+1/2}, t, u, \xi) = \frac{1}{\tau} \int_0^t g(x', t', u, \xi)e^{-(t-t')/\tau} \, dt' + e^{-t/\tau} f_0(x_{j+1/2} - ut),$$

where $x' = x_{j+1/2} - u(t - t')$ is the trajectory of a particle motion and $f_0$ is the gas distribution function at the beginning of each time step ($t = 0$). In order to evaluate $f$ at a cell interface, two unknowns, $g$ and $f_0$ in the above equation, have to be specified. The initial condition of the macroscopic variables, which is used for the construction of $g$ and $f_0$, is shown in Fig. 1. In the following, the notation $x_{j+1/2} = 0$ is used.

The initial gas distribution function $f_0$ has the form 

$$f_0 = \begin{cases} g'(1 + a'x - \tau(a'u + A')), & x \leq 0, \\ g'(1 + a'x - \tau(a'u + A')), & x \geq 0, \end{cases}$$

where $a'$ and $a''$ come from the spatial derivative of a Maxwellian distribution function and have a unique correspondence with the slopes of the conservative variables. The terms $-\tau(a'u + A')g'$ and $-\tau(a'u + A')g''$ account for the nonequilibrium parts obtained from the Chapman–Enskog expansion of the BGK model [10]. The equilibrium state $g$ around $(x = 0, t = 0)$ is assumed to have the form 

$$g = g_0(1 + (1 - H[x])a'x + H[x]a''x + \bar{A}t),$$

where $H[x]$ is the Heaviside function. Here $g_0$ is a local Maxwellian distribution function.
located at \( x = 0 \). The dependence of \( a', a', \ldots, \tilde{A} \) on the particle velocities can be obtained from a Taylor expansion of the Maxwellian, which have to be evaluated by consistently solving the BGK equation and its compatibility condition (see [10] for details).

After substituting \( f_0 \) and \( g \) into the integral solution of the BGK model, the gas distribution function \( f \) at a cell interface becomes

\[
\begin{align*}
  f(x_{j+1/2}, t, u, \xi) &= (1 - e^{-\tau t})g_0 + \tau(t/\tau - 1 + e^{-\tau t})\tilde{A}g_0 \\
  &\quad + (\tau(-1 + e^{-\tau t}) + t e^{-\tau t})(\tilde{a}'H[u] + a'(1 - H[u]))ug_0 \\
  &\quad + e^{-\tau t}((1 - u(t + \tau)a')H[u]g' + (1 - u(t + \tau)a')(1 - H[u])g') \\
  &\quad + e^{-\tau t}(-\tau A'H[u]g' - \tau A'(1 - H[u])g'),
\end{align*}
\]

from which the numerical fluxes across a cell interface can be constructed,

\[
  F_{w,j+1/2} = \int u \psi f(x_{j+1/2}, t, u, \xi) \, d\Xi.
\]

The finite-volume kinetic scheme for the update of conservative variables \( w \) in 1D case is

\[
  w_{j+1}^{n+1} = w_j^n + \frac{1}{\Delta x} \int_0^{\Delta t} \left( F_{w,j-1/2} - F_{w,j+1/2} \right) \, dt.
\]

In the above BGK method, the MUSCL-type reconstruction techniques have to be used to reconstruct the distribution of the conservative variables inside each cell at the beginning of each time step. What we propose in this note is that we can extract more information from the time-accurate gas distribution function. In the above BGK scheme, we have obtained explicitly the gas distribution function \( f \) at the cell interface (see Eq. (2)). Therefore, we can evaluate not only the fluxes from it but also the conservative flow variables there at the next time step. For example, at \((x_{j+1/2}, \Delta t)\), we can calculate the pointwise value

\[
  w_{j+1/2}^{n+1} = \begin{pmatrix} \rho \\ \rho U \\ \rho E \end{pmatrix}_{j+1/2}^{n+1} = \int \psi f(x_{j+1/2}, \Delta t, u, \xi) \, d\Xi.
\]

Note that there is no enforcement of monotonicity in the values \( w_{j+1/2}^{n+1} \) to bound it within neighboring averages. In a real physical situation, such as the collision of two shocks, the local flow variables can indeed become higher than the values in the neighboring cells. Hence, for cell \( j \) at time step \( n + 1 \), we have both the updated cell-averaged value \( w_j^{n+1} \) through Eq. (3) and the two pointwise flow variables at the left and right cell interfaces \( w_j^{n+1} \) and \( w_{j+1/2}^{n+1} \) (see Fig. 2). As a result, the slope of the conservative variables \( w \) at time level \( n + 1 \) inside cell \( j \) can be obtained from the two differences directly,

\[
  w_{x-} = 2 \left( w_j^{n+1} - w_{j-1/2}^{n+1} \right) / \Delta x, \quad w_{x+} = 2 \left( w_{j+1/2}^{n+1} - w_j^{n+1} \right) / \Delta x.
\]

For example, a single slope for the conservative variable inside cell \( j \) at time step \( n + 1 \) can
be constructed as \[3\]

\[
(dw/dx)_{j}^{n+1} = (w_{x-}|w_{x+}| + w_{x+}|w_{x-}|) / (|w_{x+}| + |w_{x-}|).
\]

The above-slope \((dw/dx)_{j}^{n+1}\) and the conservative variable \(w_{j}^{n+1}\) in Eq. (3) can be used as the initial conditions for the BGK scheme to continue the flow evolution to the next time level \(n + 2\). Therefore, the reconstruction stage with a large stencil is avoided in the current method. As an application, we tested both the previous gas-kinetic BGK scheme [10] and the newly proposed slope-update BGK scheme in two cases, i.e., the Shu–Osher shock sound wave interaction case and the Woodward–Colella blast wave case [6, 8]. Figures 3–6 show the density and velocity distributions calculated from both schemes and in both cases, where 400 grid points are used in all calculations. The solid lines are obtained from the newly proposed scheme, and the circles are the results from the previous BGK method, where the van Leer limiter is used for the initial slope reconstruction [10]. Even without using a large stencil for the slope reconstruction, the newly proposed slope-update method has less dissipation and higher accuracy than the slope-reconstruction BGK scheme. As with TVD schemes, the current method has a second-order accuracy due to the implementation of linear slopes in the initial condition and its time-dependent gas evolution. Since it calculates the conservative flow variables as well at a cell interface, it needs slightly more storage per cell than a standard MUSCL-type scheme.

In conclusion, a numerical scheme for updating the slope of the conservative variables is proposed. The success of the slope-update scheme depends solely on the temporal accuracy of the gas-evolution model, from which the accurate time-dependent conservative variables at a cell interface can be evaluated. As a result, even with the stencil of a first-order spatial accuracy scheme, a high-resolution method is constructed. From this note, we can realize the importance of keeping the temporal accuracy of a numerical scheme over using a scheme.
FIG. 3. Density distributions in the shock sound wave interaction case. Circles, MUSCL-type gas-kinetic BGK scheme with the van Leer limiter for initial slope reconstruction; solid line, slope-update scheme. In both cases 400 grid points are used. Dash–dot line, solution obtained using 1200 grid points.

FIG. 4. Velocity distributions in the shock sound wave interaction case.
FIG. 5. Density distribution in the blast wave test. Circles, MUSCL-type gas-kinetic BGK scheme with the van Leer limiter for initial slope reconstruction; solid line, slope-update scheme. In both cases 400 grid points are used. Dash–dot line, solution obtained using 1200 grid points.

FIG. 6. Velocity distributions in the blast wave case.
solely based on the high-order spatial interpolation techniques in the control of numerical dissipation.

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