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Gas-Kinetic Relaxation (BGK-Type) Schemes for the Compressible Euler Equations

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Abstract

Starting from the gas-kinetic model, a new class of relaxation schemes for the Euler equations are presented. Instead of linearizing the Euler equations into a few simple waves, the new flow solvers are based on the BGK model for the evolution of particle distribution functions, *i.e.* a nonequilibrium state will evolve into an equilibrium state along with the increasing of entropy. The numerical discretization combines naturally both the Lax-Wendroff and the Flux Vector Splitting type schemes. The numerical results for a few well-defined test cases are presented to indicate the robustness and accuracy of the BGK-type schemes.

1 Introduction

Many high resolution shock capturing schemes have been developed in the past decades. Most of them either attempt to resolve wave interactions through the upwind biasing of the discretization or explicitly introduce numerical viscosity in just the amount needed to resolve discontinuities. Generally, there are different design principles for the construction of high resolution schemes [7].

As pointed out by van Leer [20], a high resolution scheme usually consists of two parts, the re-

construction of the initial data and the dynamical evolution started from the constructed data. In other words, these two stages can be regarded as geometrical and dynamical correlations for the gas flow around an artificially defined cell boundary.

The geometrical stage is a kinematic description of the flow variables, which tries to recover the continuous physical reality from the discretized data. Caution should be taken whenever doing the interpolations. Otherwise, Gibbs phenomena or local extrema can be unphysically created. The inclusion of some kind of limiters to eliminate the creation of any "unreasonable" local extrema is physically and numerically necessary. The interpolated quantities could be continuous or discontinuous at the cell boundary according to the real flow situations: both cases are equally important. The behavior of different limiters is usually problem dependent: one limiter which is good for one test case may show unfavorable results for another one. Usually, a high-order interpolation rule does not necessarily guarantee that the final scheme will also have the same order of accuracy as the order of the interpolation, since the solutions of the model equations (such as the Euler equations) with the reconstructed data as the initial condition is also a source of error.

The second stage is the dynamical correlation, which uses physical models to construct the gas evolution picture starting from the initially interpolated data, and finally to obtain the numerical fluxes at a cell boundary. For the Euler equations, only a few exact solutions can be found for simple

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initial value problems. For example, the Riemann solver provides an exact solution under the condition of two constant states in the left and right sides of a cell boundary for 1-D gas flow, and Godunov-type schemes are based on this solution [3]. One advantage of the Godunov method is that it includes gas dynamical interactions in the time evolution process, and the flow correlations can be clearly observed from the approximate Riemann solver, such as Roe's scheme, where Roe's average is actually a constructed correlation of the flow variables between two constant states [17]. However, except under special physical situations, the flow variables are not necessarily in two constant states. Therefore, the Riemann solver is only a first-order representation of gas evolution model, and the reconstructed data in the first stage has to be abandoned in some degree in order to fit the initial value condition of the Riemann solver. Most authors, however, ignore this point, by mixing the order of the interpolation with the order of dynamics [20]. For example, van Leer points out that all one needs to do, to raise the order of accuracy of upwind differencing scheme, is to raise the order of accuracy of the initial-value interpolation that yields the zone-boundary data. Although, Godunov-type methods have been successfully used in many numerical calculations, the ability of this gas evolution model to approximate all kinds of physical processes is still doubtful [16]. In order to compensate the limitation in the Riemann solver to represent the dynamical interaction, Colella and Woodward incorporated more physical reality into their PPM scheme, where two constant states for the Riemann solver are reconstructed from the initially interpolated parabolic distribution according to the local wave speeds [2].

A numerical scheme should have both the geometrical correlation in the first stage and the dynamical correlation in the second stage, and these two stages are inseparable. The upwind property is best understood when it is applied to the simple advection equation, where the geometrical and dynamical correlations look the same. For a nonlinear system, such as the Euler equations, the story is different. To handle all conservation laws by one single method based on the linear advection equation is to try to account for all possible modes of

nonlinear interactions, which seems extremely difficult and physically unreasonable. One group of upwind schemes is Flux Vector Splitting (FVS), which are usually excessively diffusive and smear the shear layers [18, 19]. The reason for this is that FVS does not incorporate any dynamical wave interactions between the two constant states, more precisely, the left and right moving waves are formed independent of each other. For example, a right moving wave from the left state will evolve regardless of the right state. Actually, the dynamical model in FVS schemes is the collisionless Boltzmann equation. In contrast, the waves generated in Flux Difference Splitting (FDS) schemes are based on the common state at the cell interface. There are many versions of Flux Vector Splitting schemes, starting from both the Euler or gas-kinetic equations. In all these versions, if correlations between the left and right moving waves are missed in the dynamical stage, these schemes will definitely fail for Navier-Stokes simulations due to the intrinsic diffusive nature in its underlying discretized numerical model. The Advection Upstream Splitting Method (AUSM) of Liou and Steffen [11] has the correlations between the left and right states in the construction of common flow variables, such the velocity $u_{j+1/2}$ and Mach number $M_{j+1/2}$, at cell boundaries through some kind of averages. Hence, it could do an extremely good job of resolving the shear layers if the correlations are chosen properly. But in common with other upwind schemes, it could converge to non-physical solutions under some extreme conditions [21]. MacCormack and Candler also realized that the artificial dissipation in the FVS schemes could be reduced by evaluating the "splitting" at a common state [13]. Searching for better averages (or dynamical flow correlation functions) between the left and right states at a cell boundary is still under intensive investigation [12]. For central difference schemes with explicit artificial dissipation, flow interaction properties are usually obtained by the simple average of the flow variables at a cell boundary, such as the construction of the matrix $A_{i+1/2}$ in the Lax-Wendroff type schemes and the evaluation of the Euler fluxes in JST schemes [8]. This simple arithmetic average does not resemble the dynamical character of the flow either, especially in discontinuous regions.

The current state of the art design principles are referred to as Total Variation Diminishing (TVD), Essentially Nonoscillation (ENO) and Local Extremum Diminishing (LED) [4, 5, 6], which are mostly understood for the scalar conservation laws and can be applied reasonably in the reconstruction stage. In the gas evolution stage, the solution is not necessarily a decreasing function of time, and local extrema can be easily generated due to the nonlinear wave interactions.

In summary, due to the complicated nature of the Euler equations, only a few exact solutions can be constructed under very simple initial value conditions, such as the Riemann solver. Fortunately, the dynamical model to describe the gas evolution process is not unique. From the gas-kinetic BGK model, without getting into the details of the particle collisions, the time dependent solution of the gas distribution function at a cell boundary can be obtained under more flexible initial conditions, and the scheme solves the Navier-Stokes equations directly [23, 15, 24, 25]. The intrinsic physical property of upwinding is satisfied more reasonably on the level of particle motion instead of picking up a limited number of waves. In addition, the numerical solution satisfies the entropy condition naturally [25]. We define, for the first time, these kinds of schemes based on the collisional BGK model as the BGK-Type schemes in order to distinguish it from other Boltzmann-type schemes based on the collisionless Boltzmann equation in the dynamical stage.

In this paper, section 2 describes a new construction of relaxation scheme (BGK-type) for the compressible Euler equations. In contrast to previous work, the collision time does not appear in the final flux formulation, and the time evolution process is simplified [15, 24, 25]. Section 3 describes the application of this scheme to well-defined test cases.

2 Gas-Kinetic Relaxation Schemes

The fundamental task for constructing a finite-volume gas-kinetic scheme is to obtain the gas distribution function f at a cell interface, from which the numerical fluxes can be computed. For the hy-

drodynamical simulations, the behavior of the fluid depends very little on the nature of individual particle in that fluid. The most important criterion for the microscopic model is that it satisfies the minimum requirements of *conservation*, *symmetry* and *dissipation*. The BGK model satisfies all these requirements [1], from which the Euler and Navier-Stokes equations can be derived. A number of BGK-type schemes based on this model have been developed in the past few years [23, 15, 24, 25]. In this section, a further simplified gas relaxation (BGK-type) scheme for the Euler equations will be presented.

The BGK model describes the evolution of gas distribution function f . In two dimensions, the equation can be written as

$$f_t + u f_x + v f_y = (g - f)/\tau, \quad (1)$$

where g is the equilibrium state which the real gas distribution function f approaches in a time scale τ . The collision time τ is related to the local density and temperature. In the above equation, both f and g are function of space (x, y) , time t , particle velocity (u, v) and the internal variable ξ (with K degrees of freedom). The relations between the macroscopic mass ρ , momentum $\vec{P}$ and energy ϵ densities with the distribution function f are

$$\begin{pmatrix} \rho \\ P_x \\ P_y \\ \epsilon \end{pmatrix} = \int \psi_\alpha f d\Xi, \quad \alpha = 1, 2, 3, 4 \quad (2)$$

where ψ_α is the vector of the moment, defined as

$$\psi_\alpha = (1, u, v, \frac{1}{2}(u^2 + v^2 + \xi^2)) \quad (3)$$

and $d\Xi = dudvd\xi$ is the phase space volume element. The equilibrium state g , in the BGK model, is a Maxwellian distribution function, given by

$$g = A e^{-\lambda((u-U)^2 + (v-V)^2 + \xi^2)}, \quad (4)$$

here U and V are average macroscopic velocities, and λ is related to the particle mass m and temperature T through $\lambda = -m/2kT$. Since mass, momentum and energy are conservative quantities

in the process of particle collisions, f and g have to satisfy the conservation constraint of

$$\int \psi_\alpha (f - g) d\Xi = 0, \quad \alpha = 1, 2, 3, 4 \quad (5)$$

at any point in space and time.

The general solution of f from Eq.(1) can be written as

$$f(x, y, t, u, v, \xi) = \frac{1}{\tau} \int_0^t g(x', y', t', u, v, \xi) e^{-(t-t')/\tau} dt' + e^{-t/\tau} f_0(x - ut, y - vt), \quad (6)$$

where $x' = x - u(t - t')$, $y' = y - v(t - t')$ are the trajectory of a particle motion, and f_0 is the initial nonequilibrium gas distribution function f at the beginning of each time step ($t = 0$). Two unknowns g and f_0 must be determined in the above equation in order to obtain the solution f .

Due to the nonlinearity in the BGK model, shock waves and other discontinuities, whose scales are much smaller than a single cell size, are easily formed. In these regions, the gas distribution function f changes dramatically in space and stays locally in a nonequilibrium state. So, a safe representation of the initial f_0 around a cell interface is to interpolate it separately in the $x > 0$ and $x < 0$ regions. Thus, f_0 is assumed as

$$f_0 = \begin{cases} g_l, & x < 0 \\ g_r, & x > 0. \end{cases} \quad (7)$$

Both g_l and g_r are Maxwellians, which can be totally obtained from the interpolated mass, momentum and energy densities at a cell boundary [23]. This stage is identical to obtaining two constant states in the Godunov-type schemes, since the Maxwellian and local mass, momentum and energy densities have one to one correspondence.

On the other hand, the equilibrium state g around a cell boundary is assumed as

$$g = g_0(1 + a^l(1 - H(x))x + a^r H(x)x + by + \bar{A}t), \quad (8)$$

where $H(x)$ is the heaviside function and g_0 is an initial Maxwellian distribution function located at the center of a cell interface ($x = 0, y = 0, t = 0$). The dependences of a^l, a^r, b and $\bar{A}$ on the particle velocities can be found from the Taylor expansion

of a Maxwellian, which have the following form:

$$a^l = a_j^l \psi_j = a_1^l + a_2^l u + a_3^l v + a_4^l \frac{1}{2}(u^2 + v^2 + \xi^2),$$

$$a^r = a_j^r \psi_j = a_1^r + a_2^r u + a_3^r v + a_4^r \frac{1}{2}(u^2 + v^2 + \xi^2),$$

$$b = b_j \psi_j = b_1 + b_2 u + b_3 v + b_4 \frac{1}{2}(u^2 + v^2 + \xi^2),$$

$$\bar{A} = \bar{A}_j \psi_j = \bar{A}_1 + \bar{A}_2 u + \bar{A}_3 v + \bar{A}_4 \frac{1}{2}(u^2 + v^2 + \xi^2). \quad (9)$$

All parameters of $a_1^l, a_2^l, \dots, \bar{A}_4$ are local constants. Different from previous approach [15, 24, 25], the slope a^l and a^r for the equilibrium state g across a cell interface in the x-direction is assumed to be discontinuous, which is a more flexible descriptions of flows. These terms of a^l, a^r and b correspond to the spatial variation of the macroscopic variables. If the b term in Eq.(8) were ignored, the scheme would be equivalent to the direction splitting scheme, where the gas evolution in x-direction is not related to the variation of flow variables in y-direction. Since the nonequilibrium state f_0 and the equilibrium state g_0 have to satisfy the conservation constraint (Eq.(5)) at the location ($x = 0, y = 0, t = 0$), g_0 in Eq.(8) can be obtained in the following way,

$$\begin{pmatrix} \rho_0 \\ P_{0x} \\ P_{0y} \\ \epsilon_0 \end{pmatrix} = \int_{-\infty}^{+\infty} \psi_\alpha g_0 d\Xi = \int_{u>0} \psi_\alpha g^l d\Xi + \int_{u<0} \psi_\alpha g^r d\Xi. \quad (10)$$

The above mass ρ_0 , momentum P_{0x}, P_{0y} and energy ϵ_0 densities at a cell interface, similar to the Roe's average, are constructed as a dynamical averaging between the left and right states. The construction of g_0 in this way outlines a gas interaction picture, and this picture is unique in the gas-kinetic scheme. The underlying assumption for the construction of g_0 is that gas particles from the left and right sides will collapse totally and instantaneously at the cell boundary to form an equilibrium state. This assumption creates "pseudo-collisions" in the gas flow at the cell boundary, which prevents the particles from penetrating each other easily. The detailed numerical formulation can be found in [23, 26]. It can be shown that the entropy of g_0 is always larger than the entropy of f_0 in the above construction [25], which guarantees that the

dynamical system will evolve in a physically reasonable direction, and the driving force for this evolution is the difference between the equilibrium and nonequilibrium states. The BGK model tells us that the real gas distribution f will approach g_0 , but it is not necessarily equal to it.

After obtaining g_0 , the slopes of a^l, a^r in Eq.(9) can be obtained from the following equations

$$\begin{aligned} M_{ij}a_j^l &= U_i^l, & i, j &= 1, 2, 3, 4 \\ M_{ij}a_j^r &= U_i^r, & i, j &= 1, 2, 3, 4 \end{aligned} \quad (11)$$

where the summation convention is implied and the matrix M_{ij} is defined as

$$M_{ij} = \int \psi_i \psi_j g_0 d\Xi,$$

which is known after obtaining g_0 in Eq.(10). Also, U_i^l and U_i^r are the slopes for the mass, momentum and energy distributions at both sides of a cell boundary, which can be easily obtained by connecting $\rho_0, P_{0x}, P_{0y}, \epsilon_0$ with the cell averaged mass, momentum and energy densities in the left and right cells separately. The matrix M_{ij} depends only on the the flow variables $\rho_0, P_{0x}, P_{0y}, \epsilon_0$, and its inversion of getting M_{ij}^{-1} can be done analytically [23]. Similarly, the b term in Eq.(9) can be obtained from

$$M_{i,j}b_j = U_i^\perp \quad (12)$$

where $U_i^\perp$ is the slopes of mass, momentum and energy distributions in the y-direction along the cell interface. Simple central-differences with the limiter should be used to find their slopes [24].

Substituting both Eq.(7) and Eq.(8) into Eq.(6), the time-dependent f at the center of a cell interface can be obtained. Ignoring the Navier-Stokes terms [25], the integral solution can be simplified as

$$f = (1 - e^{-t/\tau})g_0 + t\bar{A}g_0 + e^{-t/\tau}f_0. \quad (13)$$

Before obtaining the unknown term $\bar{A}$ in the above equation, let's rewrite the above equation as

$$f = g_0(1 + \bar{A}t) + e^{-t/\tau}(f_0 - g_0). \quad (14)$$

From the analysis in [25], the first term on the RHS is the gas-kinetic Lax-Wendroff formulation for the

Euler equations. According to Jameson's design principle for a numerical scheme [7], the second term is the numerical dissipation. In the gas-kinetic relaxation scheme, the numerical dissipation is from the differences between the equilibrium state g_0 and nonequilibrium state f_0 . In the smooth region, the first term will dominate. When the BGK model is solved self-consistently in the smooth region [23], the unknown $\bar{A}$ in Eq.(9) can be determined from

$$\int \psi_\alpha g_0 \bar{A} d\Xi = \int \psi_\alpha g_0 (a^l u H(u) + a^r u (1 - H(u)) + vb) d\Xi \quad (15)$$

where the above equation can be expressed simply as

$$M_{ij}\bar{A}_j = \int \psi_i g_0 (a^l u H(u) + a^r u (1 - H(u)) + vb) d\Xi. \quad (16)$$

In contrast to the Riemann solver, Eq.(14) provides an alternative gas evolution picture at a cell boundary. The first term on RHS accounts for the time evolution of the equilibrium gas distribution function, and the second one is the gas-kinetic dissipation term. As we know, the shock wave is a dissipative and stable system, and its distribution function is far away from an equilibrium state. In this case, the second term should be large. However, Flux Vector Splitting schemes over emphasize the nonequilibrium property of the gas distribution [18, 19, 14]. Instead of using Eq.(14), $f = f_0$ is assumed as the gas distribution function at a cell boundary to evaluate the numerical fluxes.

In order to further simplify the gas relaxation process for the Euler calculations, $e^{-t/\tau}$ in Eq.(14) will be approximated by some physical models. Generally, we can rewrite Eq.(14) as

$$f = g_0(1 + \bar{A}t) + \mathcal{L}(\cdot)(f_0 - g_0), \quad (17)$$

where $\mathcal{L}(\cdot)$ is the relaxation parameter and should be a function of local flow variables. $\mathcal{L}(\cdot)$ determines how fast the system can be evolving into an equilibrium state.

There are many ways to construct $\mathcal{L}(\cdot)$. In this paper one choice of $\mathcal{L}(\cdot)$ is given. As we know, for shock waves, the distribution function will stay in a nonequilibrium state along with the pressure jumps

across the shock. So, the function $\mathcal{L}(\cdot)$ can be designed as a function of local pressure differences around the cell boundary $(i + 1/2)$, which is

$$\mathcal{L}(\cdot) = 1 - e^{-C_0 \min(\Delta p_1, \Delta p_2)} \quad (18)$$

where

$$\Delta p_1 = \frac{|p_{i-1,j} + p_{i+1,j} - 2p_{i,j}|}{|p_{i,j} - p_{i-1,j}| + |p_{i+1,j} - p_{i,j}|} \quad (19)$$

and

$$\Delta p_2 = \frac{|p_{i,j} + p_{i+2,j} - 2p_{i+1,j}|}{|p_{i+1,j} - p_{i,j}| + |p_{i+2,j} - p_{i+1,j}|} \quad (20)$$

The use of pressure switches were originally presented in the JST scheme [8].

The new scheme presented in this section is summarized as follows. From the interpolation of macroscopic conservative variables, according to Eq.(7), f_0 is constructed at both sides of a cell boundary, from which g_0 can be obtained (Eq.(10)). After this, a^l , a^r and b in Eq.(8) are obtained from Eq.(11) and (12) separately. Then, from Eq.(16), $\bar{A}$ is obtained in terms of a^l , a^r and b . Then, the distribution function f at the cell boundary is given in Eq.(17), and the relaxation parameter $\mathcal{L}(\cdot)$ is determined by Eq.(18). Finally, the numerical transport of mass, momentum and energy across the cell interface in x-direction in a whole time step are

$$\begin{pmatrix} \Delta \rho_0 \\ \Delta P_{0x} \\ \Delta P_{0y} \\ \Delta \epsilon_0 \end{pmatrix} = \int_0^{\Delta t} \int \psi_\alpha u f dt d\Xi, \quad (21)$$

where Δt is the CFL time step. The scheme for the y-direction fluxes can be done similarly using the procedures shown in this section.

3 Numerical Examples

Many 1-D and 2-D test cases have been presented for the numerical Euler and Navier-Stokes solutions using the earlier gas-kinetic schemes based on the solution of the BGK model [15, 24, 25]. This scheme is also being applied to the linear advection and nonlinear Burgers' equation [9]. It appears that this scheme can give very accurate results for

unsteady flow calculations, especially for problems with strong rarefaction waves in the high-speed low density regions. Actually, this is not surprising, since all particles with velocities from $-\infty$ to $+\infty$ have been considered in the process of computing numerical fluxes.

In all the following, we will apply the relaxation scheme developed in this paper to some well-known test cases with strong shocks. In all calculations, the van Leer-limiter

$$L(u, v) = S(u, v) \frac{2|u||v|}{|u| + |v|}, \quad (22)$$

with $S(u, v) = 1/2\{\text{sign}(u) + \text{sign}(v)\}$, is used for all interpolations of the macroscopic variables, and $C_0 = 1.0$ is fixed in Eq.(18).

Case(1). The first case is the blast wave test with the initial conditions $\rho_l = 1.0$, $P_l = 0$, $\epsilon_l = 2500$ for $0 < x \leq 0.1$, $\rho_m = 1.0$, $P_m = 0.0$, $\epsilon_m = 0.025$ for $0.2 < x \leq 0.9$ and $\rho_r = 1.0$, $P_r = 0.0$, $\epsilon_r = 250$ for $0.9 < x \leq 1$ [22]. 400 points are used in this case, and the results are shown in Fig.(1) for the density, velocity and pressure distributions, where the solid lines are obtained from the same scheme with 800 points.

Case(2). The forward-facing step case is carried out on a uniform mesh of 240×80 cells [22]. The density and entropy contours are shown in Fig.(2) from the full relaxation scheme presented in last section. In the case of deleting vb term in Eq.(16) when evaluating time evolution part $\bar{A}$, the original relaxation scheme (full scheme) goes back to the directional splitting scheme where the x-direction gas evolution process is independent of the flow variations in the y-direction. In this case, the density and entropy contours are shown in Fig.(3). The difference between the results from the splitting and full schemes is that the splitting scheme gives a more obvious second Mach stem on the lower surface and its amplitude of the slip line originated from the triple point close to the upper surface is less amplified. In both calculations, no special treatment around the corner is employed.

Case(3). The Mach 10 reflection of a strong shock wave over a wedge is calculated on the computational domain of 360×120 cells [22]. The problem is set up by driving a shock down a tube which contains a wedge. The density and entropy contours

are shown in Fig.(4) from the full scheme. The results from splitting scheme are shown in Fig.(5). In this case, there is almost no difference in the results from these two schemes.

All these results confirm the high accuracy of the current gas-kinetic relaxation scheme. Complex features, such as oblique shocks and the triple points, are captured without oscillations.

4 Conclusion

The gas-kinetic relaxation scheme for the Euler equations presented in this paper is a simplification of the basic idea of the BGK-Type schemes developed in the earlier papers [23, 15, 24, 25]. Different from Godunov-type schemes, this new scheme provides an alternative gas evolution model. The initial data used in the BGK-type schemes is more flexible than those used in the Riemann solver. The final time-dependent gas distribution function combines both kinetic Lax-Wendroff and Flux Vector Splitting schemes, while the difference between the nonequilibrium and equilibrium states provides a natural artificial dissipative mechanism. Due to the freedom in constructing the microscopic dynamical models for the macroscopic flow motion, a host of variations of the present scheme can be obtained by modifying the relaxation parameter $\mathcal{L}(\cdot)$. Numerical results for a few test cases demonstrate the great potential of the BGK-type schemes. A similar scheme using the distribution function

$$f = g_0(1 + \bar{A}(t - \tau) - \tau(ua'H(u) + ua^r(1 - H(u)) + vb)) + \mathcal{L}(\cdot)(f_0 - g_0)$$

for the Navier-Stokes solutions will be presented in the subsequent paper [27].

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Figure 1: Blast Wave Case with 400 points

Figure 2: Density and Entropy Distributions from Full Relaxation Scheme

Figure 3: Density and Entropy Distributions from Splitting Scheme

Figure 4: Density and Entropy Distributions from Full Relaxation Scheme

Figure 5: Density and Entropy Distributions from Splitting Scheme