A Symplectic-preserving Gas-kinetic Scheme for Hydrodynamic Equations under external forcing Field

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Abstract. In this paper, based on the BGK equation, Liouville's theorem, and symplectic preserving property of a Hamiltonian flow, a well-balanced kinetic scheme for the compressible Navier-Stokes equations under external forcing field is developed. In order to construct such a scheme, the physical process of particles transport through a potential barrier at a cell interface will be modeled with penetration and reflection according to incident particle velocity, and the symplectic property of phase space volume. For the simulation of a gravitational gas system, the current scheme has both a well-balanced property for keeping hydrostatic solution and the shock capturing capability for unsteady flow. In this paper, we will present a symplectic preserving BGK scheme with the inclusion of particle collision in the gas evolution stage. For a highly non-equilibrium flow with external forcing term, a similar scheme with the discretization of particle velocity space can be developed as well for the solution of Maxwell-Vlasov and other kinetic equations.

Keywords: gas-kinetic scheme, hydrodynamic equations, gravitational potential, symplectic preserving, well-balanced scheme
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INTRODUCTION

Generally, flows equations with source terms in one-dimensional case can be written as

$$U_t + F(U)_x = S, \tag{1}$$

where U is the vector of conservative flow variables with corresponding fluxes $F(U)$ and S is the source term. For a gas flow under an external time-independent gravitational field, there is a special hydrostatic solution with a constant temperature and zero fluid velocity. The scheme which could keep such a solution is called a well-balanced method. This solution is an intrinsic solution due to the balance between the flux gradient and source term, i.e.,

$$F(U)_x = S. \tag{2}$$

In order to develop an accurate flow solver for a slowly evolving gravitational gas dynamic system, such as the galaxy evolution problem in astrophysics, the numerical scheme should not only have the shock-capturing ability, but also be a well-balanced one.

There have been many attempts to construct well-balanced gas dynamic codes that preserve the hydrostatic solution ([4, 14, 2]). The schemes in [4, 14, 2] are designed based on the condition Eq.(2), such as to re-balance the quantities which are not in hydrostatic balance after the original updating. However, for a transition flow, the direct use of Eq.(2) in the design of the scheme is problematic, because in general case Eq.(2) cannot be enforced in a physical evolution process at all, especially for the flows around discontinuities. So, our aim of this paper is to design a general scheme with correct particle transport physics across a potential barrier, which becomes automatically a well-balanced one under the hydrostatic situation.

In the past years, gas-kinetic BGK scheme has been developed successfully for compressible Euler and Navier-Stokes equations ([10, 11]). The main part of the BGK scheme is to find the distribution function f at the cell interface, from which the numerical fluxes can be obtained and used in a finite volume method. In an early approach, a gas kinetic scheme (GKS) for gravitational system [9] has been constructed with the inclusion of particle acceleration in the transport process. The above scheme much improved the solution in comparison with operator splitting method. Unfortunately, the assumption of a continuous distribution of the gravitational potential makes the scheme in [9] not be a precise well-balanced method. Instead, in this paper we are going to approximate the gravitational potential as a

piecewise continuous function with a potential jump at the cell interface. In a previous paper [13], a first-order well-balanced kinetic flux vector splitting scheme for gravitational Euler equations has been developed. However, in the above approach, only a few simple moments of a gas distribution function are needed, and these simple moments can be intuitively guessed rather than derived from a solid physical and mathematical foundation. In order to extend the above scheme to high-order and solve the gravitational NS equations, the gas-kinetic BGK model with the inclusion of particle collision has to be solved. In developing such a scheme, much more high-order moments, i.e., up to $6th$-power of a particle velocity, have to be evaluated. It can be hardly obtained through institutive guessing. Therefore, we need to use the symplectic property of a Hamiltonian system and Liouville's theorem to evaluate high-order moment of a gas distribution function on both sides of a cell interface which is associated with a potential jump. Furthermore, to develop a scheme based on a collision model is much more challenge than that for the collision-less case. Around a potential jump, a multiple equilibrium states have to be constructed on both sides of a jump. In the construction of such an equilibrium state for the BGK model, the second law of thermodynamics has to be explicitly satisfied.

CONSTRUCTION OF SYMPLECTIC PRESERVING BGK SCHEME

The 1-D BGK scheme without external forcing field

The BGK equation without external forcing field is

$$f_t + uf_x = \frac{g-f}{\tau}, \tag{3}$$

where f is the gas distribution function and g is the equilibrium state approached by f. The particle collision time τ is related to the viscosity and heat conduction coefficients, i.e., $\tau = \mu/p$ where μ is the dynamic viscosity coefficient and p is the pressure. The relation between mass ρ, momentum ρU, and energy ρE densities with the distribution function f is

$$\begin{pmatrix} \rho \\ \rho U \\ \rho E \end{pmatrix} = \int \psi_\alpha f d\Xi, \qquad \alpha = 1,2,3, \tag{4}$$

where ψ_α is the component of the vector of moments

$$\psi = (\psi_1, \psi_2, \psi_3)^T = (1, u, \frac{1}{2}(u^2+\xi^2))^T,$$

$d\Xi = dud\xi_1 d\xi_2 ... d\xi_K$ is the volume element in the phase space. For 1D flow, the total number of degrees of freedom K in ξ is equal to $(3-\gamma)/(\gamma-1)$, and γ is the ratio of specific heat. Since mass, momentum, and energy are conserved during particle collisions, f and g satisfy the conservation constraint,

$$\int (g-f)\psi_\alpha d\Xi = 0, \qquad \alpha = 1,2,3, \tag{5}$$

at any point in space and time. The integral solution of (3) is

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

where $x' = x - u(t-t')$ is the particle trajectory. The solution f in (6) solely depends on the modeling of f_0 and g.

By using the MUSCL-type limiter, a discontinuous reconstruction for the macroscopic flow variables can be obtained around a cell interface. So, based on the Chapmann-Enskog expansion to the Navier-Stokes order, the initial gas distribution function f_0 in (6) on both sides of a cell interface can be constructed as

$$\begin{aligned} f_0^l(x,u,\xi) &= g_0^l(1 + a^l(x - x_{j+1/2}) - \tau(a^l u + A^l)), \quad x \le x_{j+1/2}, \\ f_0^r(x,u,\xi) &= g_0^r(1 + a^r(x - x_{j+1/2}) - \tau(a^r u + A^r)), \quad x > x_{j+1/2}. \end{aligned} \tag{7}$$

Here $g_0^{l,r}$ are the corresponding Maxwellians at different sides of the interface, i.e.,

$$g_0^{l,r} = \rho^{l,r}\left(\frac{\lambda^{l,r}}{\pi}\right)^{\frac{K+1}{2}} e^{\lambda^{l,r}((u-U^{l,r})^2+\xi^2)}, \tag{8}$$

where λ is equal to $m/2kT$, m is the molecular mass, k is the Boltzmann constant, and T is the temperature. The equilibrium distribution functions around the cell interface $x_{j+1/2}$ can be modeled as

$$\begin{aligned} g^l(x,t,u,\xi) &= g^l_{j+1/2}(1+\overline{a}^l(x-x_{j+1/2})+\overline{A}^l t), \quad x \le x_{j+1/2}, \\ g^r(x,t,u,\xi) &= g^r_{j+1/2}(1+\overline{a}^r(x-x_{j+1/2})+\overline{A}^r t), \quad x > x_{j+1/2}. \end{aligned} \tag{9}$$

In the case without external forcing term, $g^l_{j+1/2}$ and $g^r_{j+1/2}$ in the above equation are the same distribution functions, i.e., $g^l_{j+1/2} = g^r_{j+1/2}$, which are obtained by

$$\int g^l_{j+1/2}\psi d\Xi = \int g^r_{j+1/2}\psi d\Xi = W_{j+1/2} = \int_{u>0} f_0^l(x_{j+1/2}-ut,u,\xi)\psi d\Xi + \int_{u<0} f_0^r(x_{j+1/2}-ut,u,\xi)\psi d\Xi. \tag{10}$$

Therefore, at the cell interface the final distribution function can be fully determined using the integral solution

$$f^l(x_{j+1/2},t,u,\xi) = \frac{1}{\tau}\int_0^t g^l(x',t',u,\xi)e^{-(t-t')/\tau}dt' + e^{-t/\tau}f_0^l(x_{j+1/2}-ut), \qquad u \ge 0, \tag{11}$$

$$f^r(x_{j+1/2},t,u,\xi) = \frac{1}{\tau}\int_0^t g^r(x',t',u,\xi)e^{-(t-t')/\tau}dt' + e^{-t/\tau}f_0^r(x_{j+1/2}-ut), \qquad u < 0, \tag{12}$$

which can be used to evaluate the fluxes

$$F^l_{j+1/2}(t) = F^r_{j+1/2}(t) = \int_{u>0} uf^l(x_{j+1/2},t,u,\xi)\psi d\Xi + \int_{u<0} uf^r(x_{j+1/2},t,u,\xi)\psi d\Xi, \tag{13}$$

and update the cell averaged conservative variables

$$W_j^{n+1} = W_j^n + \frac{1}{\Delta x}\int_{t_n}^{t_{n+1}}\left[F^r_{j-1/2}(t) - F^l_{j+1/2}(t)\right]dt. \tag{14}$$

In summary, at the cell interface $x_{j+1/2}$ we can construct the equilibrium distribution functions $g^{l,r}_{j+1/2}$ from initial distribution $f_0^{l,r}$ and fluxes $F^{l,r}_{j+1/2}(t)$ from the integral solution $f^{l,r}$. Without external forcing term, all particles can transport freely across the interface. Therefore, the equilibrium states and fluxes at the interface have unique values $g^l_{j+1/2} = g^r_{j+1/2}$ and $F^l_{j+1/2}(t) = F^r_{j+1/2}(t)$. However, with the approximation of constant potential inside each cell and a jump at a cell interface, the modeling of the initial condition f_0 and equilibrium g around a cell interface has to be considered separately on both sides of the interface, but with the same mathematical formulation described in Eq.(7) and (9). In the next subsection, the determination of f_0 and g will be described.

The symplectic preserving BGK scheme

If there is an external forcing field , e.g., gravitational field, the potential $\phi(x)$ is modeled as a piecewise constant function, i.e., in jth cell $\phi(x) = \phi_j$ with a potential jump at the cell interface $x_{j+1/2}$. In this case, we have $g^l_{j+1/2} \neq g^r_{j+1/2}$ in Eq.(9). Their determination depends on the particle transport modeling. The potential jump gives a critical speed $U_c = \sqrt{|\phi_j - \phi_{j+1}|}$, which provides a threshold for the particle movement. Because of the potential jump, not all the particles colliding with the cell interface will pass through it. Some may be reflected due to less kinetic energy to overcome the potential barrier. For these particles passing through the cell interface, their momentum and energy need to be modified due to particle acceleration during the transport process. Without losing generality, we only discuss

the case for $\phi_j < \phi_{j+1}$. From the discussion of the previous subsection, we refer to the distribution function without external forcing field at the cell interface as original distribution function. It is

$$f(x_{j+1/2},t,u,\xi) = \begin{cases} f_j(x_{j+1/2},t,u,\xi), & u \geq 0, \\ f_{j+1}(x_{j+1/2},t,u,\xi), & u < 0. \end{cases} \tag{15}$$

In the following, the effect of the potential jump on the modification of the above distribution function and the determination of the corresponding equilibrium states due to the particle collisions between themselves and with the potential jump, will be studied. Starting from the above distribution function, the particle collision with the potential jump will change distribution functions to $f^l_{j+1/2}(t,u,\xi)$ and $f^r_{j+1/2}(t,u,\xi)$ at the left and right hand sides of the cell interface respectively,

$$f^l_{j+1/2}(t,u,\xi) = \begin{cases} f_j(x_{j+1/2},t,u,\xi), & u > 0, \\ \tilde{f}_j(x_{j+1/2},t,u,\xi), & 0 \geq u > -U_c, \\ \overline{f}_{j+1}(x_{j+1/2},t,u,\xi), & u \leq -U_c, \end{cases} \tag{16}$$

and

$$f^r_{j+1/2}(t,u,\xi) = \begin{cases} \overline{f}_j(x_{j+1/2},t,u,\xi), & u \geq 0, \\ f_{j+1}(x_{j+1/2},t,u,\xi), & u < 0. \end{cases} \tag{17}$$

In (16), $\tilde{f}_j$ is the reflected particle in the jth cell, whose original distribution function is f_j with positive velocity being less than U_c. $\overline{f}_{j+1}$ is the particles in the jth cell coming from the distribution f_{j+1} of the $(j+1)th$ cell with negative velocity. Here $\overline{f}_j$ is the particles in the $(j+1)th$ cell coming from jth cell with original velocity being higher than U_c. So, the effect of the potential jump modifies the distribution function, but the moments of the modified and original distribution functions are related through the following physical principles.

With the original particle distribution function $f(u)$, after impacting on the potential jump, the particle velocity u is changed to u' and the distribution function becomes $\overline{f}(u')$. Since the energy conservation for a particle movement under a conservative potential field, the Hamiltonian function H of the particle keeps a constant

$$H(t) = \frac{1}{2}u(t)^2 + \phi(x(t)) = constant \rightarrow \frac{1}{2}u^2 + \phi = \frac{1}{2}(u')^2 + \phi', \tag{18}$$

from which the relation between u and u' can be obtained. Also, Liouville's theorem states that the probability density of particle in phase space keeps a constant along their movement trajectory,

$$\overline{f}(u') = f(u). \tag{19}$$

Most importantly, the symplectic preserving property of the Hamiltonian phase flow shows

$$\int\int_{D'} dx'du' = \int\int_{D} dxdu, \tag{20}$$

where D' and D are the phase volume on the trajectory of the Hamiltonian phase flow. Based on $D = (u_1,u_2)\times(u_1t,u_2t)$ and $D' = (u'_1,u'_2)\times(u'_1t,u'_2t)$, Eq.(20) goes to

$$\int_{u'_1}^{u'_2} u'du' = \int_{u_1}^{u_2} udu. \tag{21}$$

Then from (19), (21) and (18),

$$n\text{th-order } u \text{ moment} = \int_{u'_1}^{u'_2} \overline{f}(u')(u')^n du' = \int_{u_1(u'_1)}^{u_2(u'_2)} f(u)(u'(u))^{n-1}udu. \tag{22}$$

So, using $f_j = f^l_0$ and $f_{j+1} = f^r_0$, we can get the conservative variables at different sides of an interface

$$W^l_{j+1/2} = \int f^l_{j+1/2}\psi d\Xi, \quad \text{and} \quad W^r_{j+1/2} = \int f^r_{j+1/2}\psi d\Xi.$$

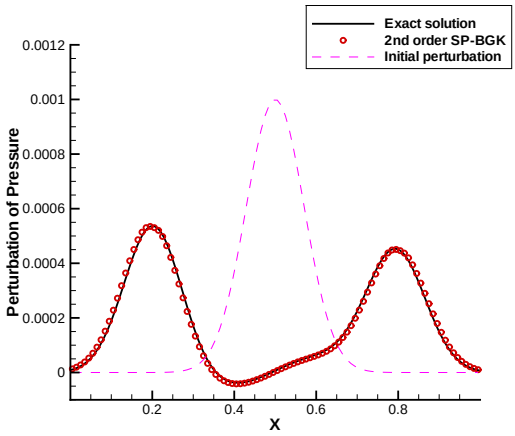

FIGURE 1. Perturbation of pressure of isothermal equilibrium solution for $\eta = 0.001$.

From which, two Maxwellians $g^l_{j+1/2}$ and $g^r_{j+1/2}$ in the equilibrium states (9) can be fully determined. Then, following the method used in the development of BGK-NS scheme [11], the final gas distribution at the left and right hand sides of a cell interface, i.e., f^l and f^r in (12), can be obtained. If choosing $f_j = f^l$ and $f_{j+1} = f^r$, we can get the corresponding fluxes at different sides of the cell interface,

$$F^l_{j+1/2} = \int u f^l_{j+1/2} \psi d\Xi, \quad \text{and} \quad F^r_{j+1/2} = \int u f^r_{j+1/2} \psi d\Xi.$$

Note that with the potential jump, in general we have $g^l_{j+1/2} \neq g^r_{j+1/2}$ and $F^l_{j+1/2} \neq F^r_{j+1/2}$. Finally, we can use (14) to update the cell average conservative variables.

NUMERICAL EXAMPLES

Perturbation of the 1D isothermal equilibrium solution: This test case is from LeVeque and Bale's paper [4]. We consider an ideal gas with $\gamma = 1.4$ on an initial isothermal hydrostatic state, $\rho_0(x) = p_0(x) = e^{-x}$, and $u_0(x) = 0$, for $x \in [0,1]$. Initially, the pressure is perturbed by $p(x,t=0) = p_0(x) + \eta e^{\alpha(x-x_0)^2}$, where $\alpha = 100$, $x_0 = 0.5$ and η is the amplitude of the perturbation. The computation is conducted with 100 grid points in the whole domain and stops at time $t = 0.25$. The potential jump at each cell interface is $\Delta\phi = -G\Delta x = 0.01$. Fig. 1 shows the result for the case $\eta = 0.001$.

Rayleigh-Taylor instability: This test case also comes from [4]. Consider an isothermal equilibrium idea gas ($\gamma = 1.4$) in a 2D polar coordinate,

$$\rho_0(r) = e^{-\alpha(r+r_0)}, p_0(r) = \frac{1.5}{\alpha} e^{-\alpha(r+r_0)}, u_0 = 0,$$

where

$$\begin{cases} \alpha = 2.68, r_0 = 0.258, & r \le r_1, \\ \alpha = 5.53, r_0 = -0.308, & r > r_1. \end{cases} \qquad \begin{cases} r_1 = 0.6(1 + 0.02\cos(20\theta)) & \text{for density} \\ r_1 = 0.62324965 & \text{for pressure.} \end{cases}$$

The potential satisfies $-\nabla\phi(r) = 1.5$. The results at times $t = 0, 0.8, 1.4$ and 2.0 are shown in fig. 2.

CONCLUSION

In this paper, based on Liouville's theorem and symplectic preserving property of a Hamiltonian flow, a kinetic scheme has been developed for the gas dynamic equations under external forcing field, where the potential is approximated as

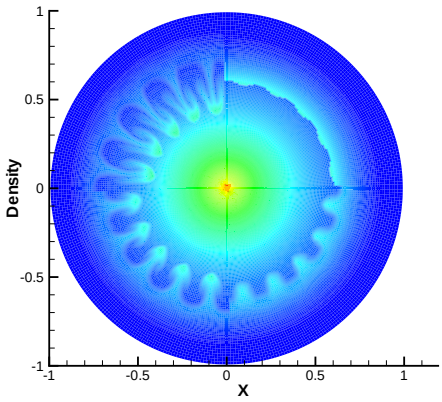

FIGURE 2. Rayleigh-Taylor instability at time t=0, 0.8, 1.4, 2.0.

a step function at the cell interface. The physical mechanism of particle transport across the potential barrier has been explicitly used in the construction of gas distribution function. The method presented in this paper is a well-balanced and shock-capturing scheme for the Navier-Stokes equations under external forcing field. The design of the scheme is based on principles of physics, instead of directly using the well-balanced condition as a guideline in the construction of such a scheme.

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