

A Well-Balanced Kinetic Scheme for Gas Dynamic Equations under Gravitational Field

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Received 07 July 2009; Accepted (in revised version) 18 September 2009

Available online 5 March 2010

Abstract. In this paper, a well-balanced kinetic scheme for the gas dynamic equations under gravitational field is developed. In order to construct such a scheme, the physical process of particles transport through a potential barrier at a cell interface is considered, where the amount of particle penetration and reflection is evaluated according to the incident particle velocity. This work extends the approach of Perthame and Simeoni for the shallow water equations [Calcolo, 38 (2001), pp. 201-231] to the Euler equations under gravitational field. For an isolated system, this scheme is probably the only well-balanced method which can precisely preserve an isothermal steady state solution under time-independent gravitational potential. A few numerical examples are used to validate the above approach.

AMS subject classifications: 35L40, 70H05, 76P05

Key words: Gas-kinetic scheme, gas dynamic equations, gravitational potential.

1 Introduction

In order to develop an accurate flow solver for a slowly evolving gas dynamic system under gravitational field, the numerical scheme has to be a well-balanced one. For example, most astrophysical problems are related to the hydrodynamical evolution in a gravitational field, a correct implementation of the gravitational force in an astrophysical hydrodynamical code is essential to capture the long time evolution in the modeling star and galaxy formation. Even though many hydrodynamical codes have been successfully applied to astrophysical problems, including the Piecewise Parabolic Method (PPM) and Total Variation Diminishing (TVD) codes [2, 5], most

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have considered only short time evolutions with strong shock or expansion waves. With the slowness of galaxy evolution, many codes have difficulties due to the improper treatment of the gravitational force effect, the so-called source term in the Euler or the Navier-Stokes equations. A simple example to check the validity of the code is to test for an isolated gas system under time-independent gravitational field. Will the solution settle down to an isothermal steady state solution? Most times, the solution will either oscillate around the equilibrium state, or simply deviate from equilibrium one due to artificial heating, which triggers numerical gravitation-thermal instability, i.e., the collapse of the gas core. There have been many attempts to construct such a well-balanced gas dynamic code that preserves the hydrostatic solution accurately [1, 3, 9].

In an earlier approach, we have developed an accurate scheme for the Navier-Stokes equations under gravitational field [6], where the flux function across a cell interface has explicitly taken into account the gravitational forcing on the particle transport. Even though the scheme is very accurate in comparison with operator splitting methods, its inadequate representation of an exact exponential density distribution inside each cell makes it not be a well-balanced one. In this paper, instead of using continuous approximation of a gravitational potential, a constant gravitational potential inside each cell with a potential jump at a cell interface is adopted. With the inclusion of the particle transport mechanism, such as penetration and reflections, a well-balanced gas-kinetic scheme for the gas dynamic equations can be developed. The development of the current method is motivated by the research work of Perthame and Simeoni [4], where the shallow water system was considered. The scheme presented in this paper is probably the only scheme which is a well-balanced one for the Euler equations under the gravitational field. Theoretically, with the piecewise discontinuous potential approximation, a well-balanced BGK-NS scheme can be constructed to solve the Navier-Stokes equations under gravitational field as well with the consideration of particles transport mechanism across a potential jump at a cell interface [8].

2 Kinetic equation for flow system with gravitational source term

In this section, we are going to present the transition from the development of a well-balanced scheme for the shallow water equations to the gas dynamic equations. It is certainly true that for the shallow water equations, there are many well-balanced schemes. The current approach is just one of the successful methods. However, the shallow water equations are much simpler than the gas dynamic equations. For the gas dynamic equation, the method presented here is probably unique in the designing of a well-balanced scheme.

For hydrostatic flows, a proper representation of the hydrostatic balance for the gas dynamic equations is critically important for slowly evolving system under gravitational field. The difficulty associated with this kind of system is the source term

treatment [1,3]. Outstanding examples are the shallow water equations,

$$h_t + (hU)_x = 0, \quad (2.1a)$$

$$(hU)_t + (hU^2 + \frac{1}{2}Gh^2)_x + h\Phi_x = 0, \quad (2.1b)$$

where G is gravitational constant and $\Phi_x = GB'(x)$ is the potential with bottom height $B(x)$, and the gas dynamic equations,

$$\rho_t + (\rho U)_x = 0, \quad (2.2a)$$

$$(\rho U)_t + (\rho U^2 + P)_x + \rho\Phi_x = 0, \quad (2.2b)$$

$$(\rho E)_t + ((\rho E + P)U)_x + \rho U\Phi_x = 0, \quad (2.2c)$$

where Φ is the gravitational potential.

In order to recover the above macroscopic equations from the gas-kinetic theory, the kinetic equation can be written as

$$f_t + uf_x - \Phi_x f_u = Q, \quad (2.3)$$

where f is the gas distribution function, u is the particle velocity, Φ is the external gravitational potential, and Q is the particle collision term. An equilibrium state for the kinetic equation should be obtained based on the requirement of $Q = 0$. However, the equilibrium state and the well-balanced solution for the hyperbolic system with source terms are two different concepts.

The equilibrium states g for the shallow water equations have to recover Eq. (2.1) through the following moments equations for the kinetic model (2.3),

$$\left(\int \psi g du \right)_t + \left(\int \psi u g du \right)_x - \Phi_x \int \psi g_u = 0, \quad (2.4)$$

with the conservative moments $\psi = (1, u)^T$. The moments of the collision term disappear automatically due to the mass and momentum conservation during the collision process. For the shallow water equations (2.1), due to its pseudo-kinetic modeling the corresponding equilibrium states may not be unique. For example, both of the following equilibrium states satisfy both Eqs. (2.1) and (2.4) precisely. One is the equilibrium state of Perthame and Simeoni [4],

$$g_1 = \sqrt{h} \frac{\sqrt{2}}{\pi \sqrt{G}} \left[1 - \frac{(u-U)^2}{2Gh} \right]^{\frac{1}{2}}, \quad \text{for } U - \sqrt{2Gh} < u < U + \sqrt{2Gh}, \quad (2.5)$$

and the other is the Maxwellian [7]

$$g_2 = \left(\frac{h}{G\pi} \right)^{\frac{1}{2}} \exp \left[-\frac{1}{Gh} (u-U)^2 \right]. \quad (2.6)$$

Therefore, the choice of a correct equilibrium state has to depend on other conditions as well, such as the recovering of viscous terms or keeping a specific well-balanced solution.

The shallow water equations (2.1) have a special solution

$$U(x, t) = 0, \quad h(x, t) + B(x) = \text{constant}. \quad (2.7)$$

Any scheme which can preserve the above solution is commonly called a well-balanced scheme. In terms of kinetic equation (2.3), the well-balanced condition (2.7) becomes

$$U = 0, \quad u g_x - \Phi_x g_u = 0, \quad (2.8)$$

for the equilibrium state. With the satisfaction of condition Eq. (2.8), for the shallow water equations the equilibrium state has to be g_1 in (2.5). If the condition changes to recover the dissipative term for the viscous shallow water equations, g_2 will be the choice.

For the well-balanced kinetic condition (2.8), a general solution is

$$g(x, u) = \chi\left(\Phi(x) + \frac{1}{2}u^2\right), \quad (2.9)$$

where χ is an arbitrary function. The above general solution reveals a fundamental physical fact that for each individual particle movement, the total energy

$$\Phi(x) + \frac{1}{2}u^2,$$

keeps a constant. This condition is precisely used in the development of a well-balanced kinetic scheme by Perthame and Simeoni for the shallow water equations [4]. In this paper, we are going to use the same physical reality to design a well-balanced scheme for the gas dynamic equations.

For the gas dynamic equations (2.2), one of the simplest well-balanced condition is to keep the isothermal hydrostatic solution

$$U(x, t) = 0, \quad \rho(x, t) = A \exp[-\alpha\Phi(x)], \quad (2.10)$$

where A and α are constants. In order to satisfy the above condition, the kinetic equilibrium state g has to be proportional to $g \sim \exp[-\alpha\Phi(x)]$. Therefore, the well-balanced kinetic condition (2.9) requires the equilibrium state to be an exact Maxwellian distribution function. This is different from the shallow water case. Based on the Maxwellian distribution function, a well-balanced scheme for the gas dynamic equation will be developed. The energy conservation condition for the particle transport,

$$\Phi(x) + \frac{1}{2}u^2 = \text{constant}, \quad (2.11)$$

will be used in designing such a scheme.

3 Well-balanced kinetic scheme for gas dynamic equations

For a finite volume scheme, the computational domain is divided into numerical cells with the cell center x_j and cell interface $x_{j+1/2}$. The conservative variables $(\rho, \rho U, \rho E)_j$ are the cell averaged quantities. For the 1st-order scheme, the potential $\Phi(x)$ inside each cell keeps a constant Φ_j , and there exists a jump from Φ_j to Φ_{j+1} at the cell interface $x_{j+1/2}$. Therefore, in order to evaluate the fluxes across the cell interface, the potential jump has to be taken into account through the total particle energy conservation (2.11). The potential jump will be associated with the particle velocity jump.

For the gas dynamic equations, the equilibrium Maxwellian distribution function has the form

$$g = \rho \left(\frac{\lambda}{\pi} \right)^{\frac{K+1}{2}} e^{-\lambda [(u-U)^2 + \zeta^2]},$$

where ρ is the density, U is the macroscopic flow velocity, and $\lambda = m/2kT$ with the molecular mass m , the Boltzmann constant k , and the temperature T . The total number of degrees of freedom K in ζ is equal to $(3 - \gamma)/(\gamma - 1)$. For example, for a diatomic gas with $\gamma = 7/5$, K is equal to 4 to account for the particle motion in the y and z -directions and two rotational degrees of freedom. In the equilibrium state, the internal variable ζ^2 is equal to

$$\zeta^2 = \zeta_1^2 + \zeta_2^2 + \dots + \zeta_K^2.$$

The relation between mass ρ , momentum ρU , and energy ρE densities with the distribution function g is

$$\begin{pmatrix} \rho \\ \rho U \\ \rho E \end{pmatrix} = \int \psi_\alpha g d\Xi, \quad \alpha = 1, 2, 3, \quad (3.1)$$

where

$$\psi_\alpha = \left[1, u, \frac{1}{2}(u^2 + \zeta^2) \right]^T.$$

All parameters in g can be determined from the cell averaged macroscopic variables, i.e., $\lambda = \rho/(2p)$, where p is the pressure.

Based on the potential jump around a cell interface, we can define a critical particle speed U_c . Only these particles with velocity being larger than the critical speed can pass through the potential barrier. Therefore, the lost momentum and energy from one cell, i.e., j , will not be equal to the amount received in the neighboring cells, i.e., $j \pm 1$. So, at each cell interface $x_{j+1/2}$, two fluxes $F_{j+1/2}^{L,R}$ on the left and right hand sides of a cell interface have to be defined. Due to the potential jump, the lost momentum and energy from cell j may not be equal to the received ones in cell $j + 1$, i.e., $F_{j+1/2}^L \neq F_{j+1/2}^R$.

Now let us consider the following two cases.

Case (1): $\Phi_j < \Phi_{j+1}$

Define a critical speed

$$U_c = \sqrt{2(\Phi_{j+1} - \Phi_j)} > 0.$$

Based on the condition (2.11), the fluxes at $x_{j+1/2}$ on the left side of the cell interface can be calculated as

$$\begin{aligned} F_{j+\frac{1}{2}}^L &= \int_{U_c}^{\infty} g_j u \begin{pmatrix} 1 \\ u \\ \frac{1}{2}(u^2 + \zeta^2) \end{pmatrix} dud\zeta + \int_0^{U_c} g_j u \begin{pmatrix} 0 \\ 2u \\ 0 \end{pmatrix} dud\zeta \\ &\quad + \int_{-\infty}^0 g_{j+1} u \begin{pmatrix} 1 \\ -\sqrt{u^2 + U_c^2} \\ \frac{1}{2}(u^2 + U_c^2 + \zeta^2) \end{pmatrix} dud\zeta, \end{aligned}$$

where the first term on the right hand side accounts for the particle penetration through the potential barrier and only these particles with velocity being larger than U_c can penetrate through the interface from cell j to $j + 1$. Those particles with speed being less than U_c will be reflected back from the interface and stay inside cell j , which is the second term on the right hand side. The last term on the right hand side presents these particles move from cell $j + 1$ to cell j . Due to the potential jump, these particles will get accelerated to a new velocity after crossing the interface.

Similarly, on the right hand side of the cell interface, the fluxes become

$$F_{j+\frac{1}{2}}^R = \int_{U_c}^{\infty} g_j u \begin{pmatrix} 1 \\ \sqrt{u^2 - U_c^2} \\ \frac{1}{2}(u^2 - U_c^2 + \zeta^2) \end{pmatrix} dud\zeta + \int_{-\infty}^0 g_{j+1} u \begin{pmatrix} 1 \\ u \\ \frac{1}{2}(u^2 + \zeta^2) \end{pmatrix} dud\zeta.$$

Case (2): $\Phi_j > \Phi_{j+1}$

Define a critical velocity

$$U_c = \sqrt{2(\Phi_j - \Phi_{j+1})} > 0.$$

The corresponding fluxes become

$$F_{j+\frac{1}{2}}^L = \int_0^{\infty} g_j u \begin{pmatrix} 1 \\ u \\ \frac{1}{2}(u^2 + \zeta^2) \end{pmatrix} dud\zeta + \int_{-\infty}^{-U_c} g_{j+1} u \begin{pmatrix} 1 \\ -\sqrt{u^2 - U_c^2} \\ \frac{1}{2}(u^2 - U_c^2 + \zeta^2) \end{pmatrix} dud\zeta,$$

and

$$\begin{aligned} F_{j+\frac{1}{2}}^R &= \int_0^{\infty} g_j u \begin{pmatrix} 1 \\ \sqrt{u^2 + U_c^2} \\ \frac{1}{2}(u^2 + U_c^2 + \zeta^2) \end{pmatrix} dud\zeta + \int_{-\infty}^{-U_c} g_{j+1} u \begin{pmatrix} 1 \\ u \\ \frac{1}{2}(u^2 + \zeta^2) \end{pmatrix} dud\zeta \\ &\quad + \int_{-U_c}^0 g_{j+1} u \begin{pmatrix} 0 \\ 2u \\ 0 \end{pmatrix} dud\zeta. \end{aligned}$$

Based on the above defined fluxes, the update of the mass, momentum, and energy inside each cell becomes

$$W_j^{n+1} = W_j^n + \frac{\Delta t}{\Delta x} (F_{j-\frac{1}{2}}^R - F_{j+\frac{1}{2}}^L).$$

The above scheme can be easily extended to second-order accuracy using MUSCL-type approach, such as reconstructing the mass, momentum, and energy inside each cell with nonlinear limiters. Then, a spatial variational gas distribution functions can be obtained, from which the particle transport across the cell interface can be evaluated similarly by taking into account the potential jump.

For a well-balanced hydrostatic solution with

$$U_j = 0, \quad \lambda_j = \text{constant}, \quad \text{and} \quad \rho_j = A \exp(-\lambda_j \Phi_j),$$

it can be proved mathematically that the above scheme can precisely preserve such a solution. Due to the intrinsic dissipation in the kinetic scheme, for an isolated system with stationary adiabatic boundary condition, any physically realizable initial state will evolve into an isothermal hydrostatic solution by the current scheme.

4 Examples

Two test cases are presented in this section. The first one is the standard Sod test under gravitational potential field with reflection boundary condition. In the computational domain $x \in [0, 1]$, 100 cells are used. The initial condition is

$$(\rho = 1.0, \quad U = 0.0, \quad p = 1.0), \quad \text{for} \quad x \leq 0.5,$$

and

$$(\rho = 0.125, \quad U = 0.0, \quad p = 0.1), \quad \text{for} \quad x > 0.5.$$

The gravitational force G takes a value $G = -1.0$ in the x -direction. So, the potential jump at each cell interface becomes

$$\Delta\Phi = -G\Delta x = -0.01.$$

The computational results at $t = 0.2$ are presented in Figs. 1-3 for the density, pressure and velocity from both 1st and 2nd-order schemes. Besides the shock, contact, and rarefaction waves, the density distribution inside the tube is pulling back in the negative x -direction due to the gravitational force. In some area, the flow velocity becomes negative.

The second test case is also in a computational domain $x \in [0, 1]$ with 50 cells. There are limited number of gravitational potential jumps located at $x = 0.21, 0.41, 0.61,$ and 0.81 with a value $\Delta\Phi = 2.0$. The initial flow condition inside the domain has constant values of $\rho = 1.0, \rho U = 0.0,$ and $\rho E = 2.5$. After a long time integration,

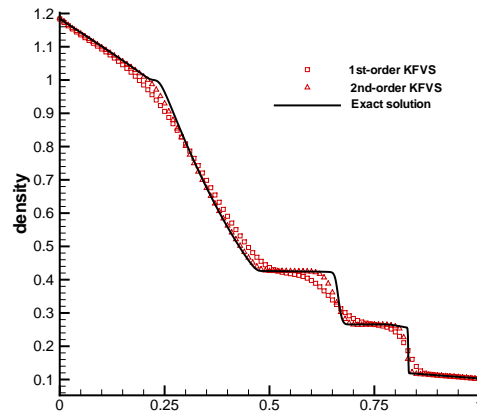


Figure 1: Density distribution for the shock tube problem under gravitational field.

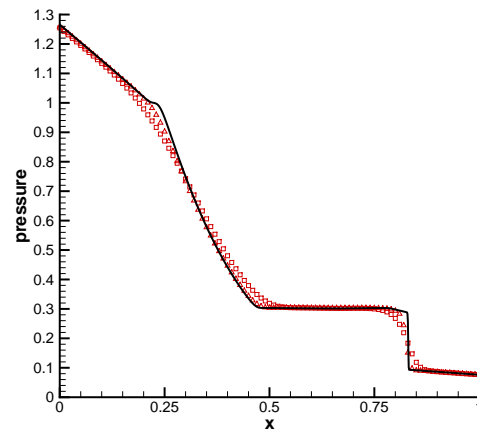


Figure 2: Pressure distribution for the shock tube problem under gravitational field.

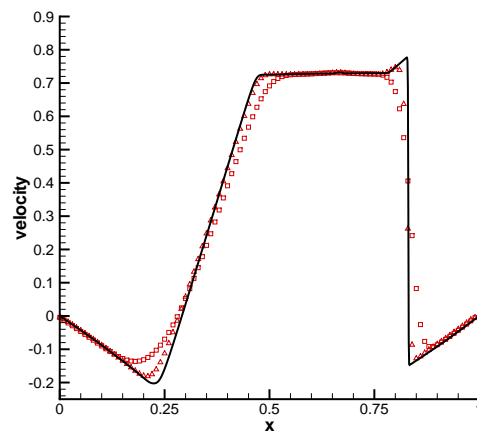


Figure 3: Velocity distribution for the shock tube problem under gravitational field.

the flow distributions settle down into a piecewise constant states shown in Fig. 4, where the symbols are the numerical solutions and the solid lines are the exact hydrostatic solutions. The gas settles to an isothermal solution and the relative temperature differences among different piecewise constant states are on the order

$$\Delta \frac{T}{T} = 10^{-5}.$$

The velocity distribution is shown in Fig. 5, where except at the potential jump locations the flow velocities at other places are on the order of 10^{-15} . If better accuracy can be achieved for the numerical evaluation of the integrals in the fluxes, the velocity error around the potential jump can be further reduced to machine zero.

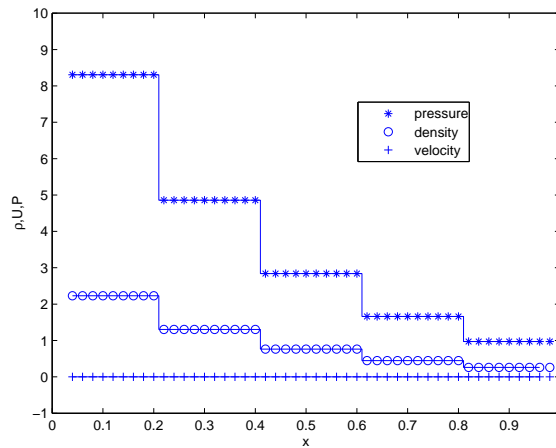


Figure 4: The converged hydrostatic solution for an isolated system with potential jumps at discrete locations. The solid lines are the exact solutions.

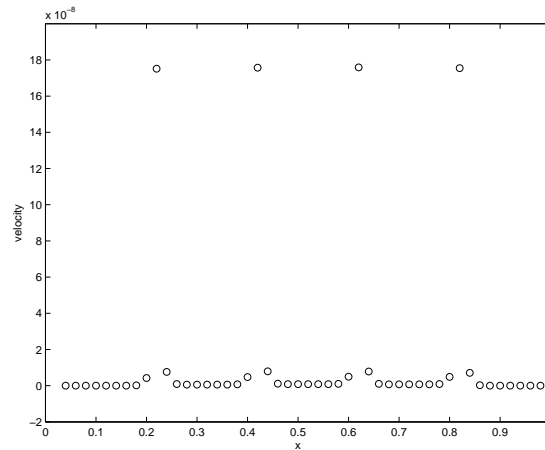


Figure 5: Velocity distribution in a steady hydrostatic state. The small velocity variation is due to the inaccurate numerical evaluation of the flux integral. There is no exact solution for the integral, which has to be calculated numerically.

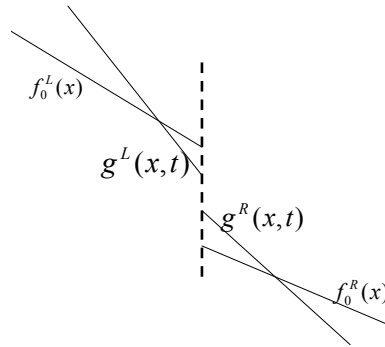


Figure 6: The gas distribution functions for the BGK-NS scheme under gravitational potential jump.

5 The extension to the Navier-Stokes equations

For the Navier-Stokes equations, instead of solving the collision-less Boltzmann equation presented in the previous sections, the collisional one, such as the BGK model, has to be solved in the gas evolution stage in order to have an appropriate representation of physical viscosity [8]. Due to the potential jump at a cell interface, both the initial gas distribution function f_0 and the equilibrium states g will become discontinuous at a cell interface, see Fig. 6. The reconstruction of f_0 can be done in the same way as the BGK-NS method [8]. However, for the equilibrium ones, we have to reconstruct them separately at the left and right sides of a cell interface with the account of particle collisions from these particles which can really get there from the same cell or from the neighboring cells through a potential jump. At the same time, the integral solutions of the BGK model will be used separately on the left and right hand sides of the cell interface to determine the time evolution part in the equilibriums states and to evaluate the final real gas distribution functions there. With the determination of the gas distribution function

$$f^l(x = x_{j+1/2}, t), \quad \text{and} \quad f^r(x = x_{j+1/2}, t),$$

at a cell interface, the numerical fluxes across the cell interface can be evaluated in the same way as that presented in section 3 with the consideration of a potential jump. Different from the collision-less approach or KFVS method, the particle collisions have been taken into account in the evaluation of the equilibrium states and their time evolutions in the collisional BGK scheme for the Navier-Stokes equations.

6 Conclusions

This paper presents a well-balanced kinetic flux vector splitting method for the gas dynamic equations under gravitational field and the potential is approximated as a

step function at each cell interface. In order to design such a scheme, the equilibrium state used has to be an exact Maxwellian distribution function. At the same time, the physical mechanism of particle transport across the potential barrier has to be explicitly used in the flux evaluation. If the gravitational potential is approximated as a continuous function in space, for the isothermal hydrostatic steady state solution the density distribution will become an exponential function. Currently, there is no computational fluid dynamics method which could explicitly follow the time evolution from an initial exponential density distribution. Therefore, there is basically no well-balanced scheme for the gas dynamic equations in the general case. With the piecewise constant approximation for the potential, the method presented in this paper is the first well-balanced scheme for the Euler equations under gravitational field. This method can be also extended to develop a well-balanced gas-kinetic scheme for the Navier-Stokes equations with gravitational source term.

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