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Higher Order Approximation Methods for the Boltzmann Equation

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A higher order time differencing method for the spatially nonhomogeneous Boltzmann equation is derived from the integral form of the equation along its characteristic line. Similar to the splitting method, which solves the collisionless equation in the convection step and the spatially homogeneous Boltzmann equation in the collision step, the present method consists of two steps, one of which is the same as the convection step in the splitting method. The difference from the splitting method is in the other step, where not only the collision term but also its variation along the characteristic line is taken into account correctly. The truncation error of this method per time step Δt is $O(\Delta t^3)$ and its higher order accuracy is demonstrated numerically in the shock propagation problem using the BGK model equation. It is shown that such accuracy is never realized in the framework of the conventional splitting formulation, which is contrary to Bogomolov's result (*U.S.S.R. Comput. Math. Math. Phys.* **28**, 79 (1988)). The other higher order methods based on the integral form are also presented. Furthermore, the extension to the stochastic approach, modification of the conventional direct simulation Monte-Carlo procedure, is proposed.

Key Words: Boltzmann equation; finite difference method; DSMC method; higher order accuracy.

I. INTRODUCTION

The splitting method is widely used in the numerical analysis of the Boltzmann equation. This method consists of two steps, i.e. the convection step, which solves the collisionless equation, and the collision step, which solves the spatially homogeneous Boltzmann equation. The direct-simulation Monte-Carlo (DSMC) method [1–3], which is the most prevailing method for predicting the behavior of rarefied gas flows at the present time, is also based on this formulation. According to Bogomolov [4], the truncation error of the splitting method per time step Δt would be $O(\Delta t^3)$ if both of these equations were solved

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exactly, which gives a sufficient reason to look for a more accurate approximation method in the framework of this formulation (see Refs. [2, 5], where the improvement of the DSMC method is mentioned in connection with Bogomolov's result). In particular, the improvement of the deterministic approach seems to be very promising, since it is expected that a higher order interpolation formula and an accurate approximation method for ordinary differential equations (e.g., the modified Euler method and the Runge-Kutta method) work well in the convection step and the collision step, respectively.

Bogomolov's illuminating result is, however, incorrect and the above expectation is an illusion; higher order accuracy is never realized in the framework of the conventional splitting formulation.

In the present study, we derive higher-order approximation methods for the time-dependent and spatially nonhomogeneous Boltzmann equation from the integral form of the equation along its characteristic line. We first reexamine the accuracy of the splitting method in Section II, where it is shown that the truncation error per time step Δt is not $O(\Delta t^3)$ but $O(\Delta t^2)$; the splitting method is first-order accurate in Δt (the error becomes $O(\Delta t)$ at $t = t_0 (= n\Delta t)$ because of the accumulation over $n (= t_0/\Delta t)$ steps). As a by-product of the error analysis, a higher order time differencing method is derived. This is presented in Section III. Similar to the splitting method, this method consists of two steps, one of which is the same as the convection step in the splitting method. In the other step, however, not only the collision term but also its variation along the characteristic line is taken into account correctly. From the integral form along its characteristic line, several higher order schemes are derived. Some of them are also presented. In Section IV, the higher order accuracy of these methods is demonstrated numerically in the shock propagation problem using the BGK model equation. Furthermore, in Section V, the extension of higher order deterministic methods to the stochastic approach is proposed.

II. ACCURACY OF SPLITTING METHOD

We examine the accuracy of the splitting method for the full Boltzmann equation in the initial-value problem,

$$\frac{\partial f(\boldsymbol{X}, \boldsymbol{\xi}, t)}{\partial t} + \boldsymbol{\xi} \cdot \frac{\partial f(\boldsymbol{X}, \boldsymbol{\xi}, t)}{\partial \boldsymbol{X}} = Q(f(\boldsymbol{X}, \boldsymbol{\zeta}, t),\, f(\boldsymbol{X}, \boldsymbol{\zeta}, t))[\boldsymbol{\xi}], \quad 0 < t \le \Delta t, \tag{1a}$$

$$f(\boldsymbol{X}, \boldsymbol{\xi}, 0) = f_0(\boldsymbol{X}, \boldsymbol{\xi}), \tag{1b}$$

where $\boldsymbol{X}$ and $\boldsymbol{\xi}$ are the position and velocity vectors in $\boldsymbol{R}^3$, t is the time, and $f(\boldsymbol{X}, \boldsymbol{\xi}, t)$ is the velocity distribution function of gas molecules. The collision operator Q is defined by

$$Q(F(\boldsymbol{\zeta}), G(\boldsymbol{\zeta}))[\boldsymbol{\xi}] = \frac{1}{2} \int (F(\boldsymbol{\xi}')G(\boldsymbol{\xi}_*') + F(\boldsymbol{\xi}_*')G(\boldsymbol{\xi}') - F(\boldsymbol{\xi})G(\boldsymbol{\xi}_*) - F(\boldsymbol{\xi}_*)G(\boldsymbol{\xi})) \times B(|\boldsymbol{V} \cdot \boldsymbol{n}|, V) d\Omega(\boldsymbol{n}) d\boldsymbol{\xi}_*, \tag{2a}$$

$$\boldsymbol{\xi}' = \boldsymbol{\xi} + \boldsymbol{n}(\boldsymbol{V} \cdot \boldsymbol{n}), \quad \boldsymbol{\xi}_*' = \boldsymbol{\xi}_* - \boldsymbol{n}(\boldsymbol{V} \cdot \boldsymbol{n}), \tag{2b}$$

$$\boldsymbol{V} = \boldsymbol{\xi}_* - \boldsymbol{\xi}, \quad V = |\boldsymbol{V}|, \tag{2c}$$

where $\boldsymbol{n}$ is a unit vector, B is a nonnegative function, the functional form of which depends on the intermolecular force law, and the domain of integration with respect to $\boldsymbol{\xi}_*$ and that with respect to $\boldsymbol{n}$ are the whole velocity space and all direction, respectively.

In the splitting method, problem (1) is divided into two steps,
convection step,

$$\frac{\partial h_1(\boldsymbol{X},\boldsymbol{\xi},t)}{\partial t}+\boldsymbol{\xi}\cdot\frac{\partial h_1(\boldsymbol{X},\boldsymbol{\xi},t)}{\partial \boldsymbol{X}}=0,\quad 0<t\le\Delta t, \tag{3a}$$

$$h_1(\boldsymbol{X},\boldsymbol{\xi},0)=f_0(\boldsymbol{X},\boldsymbol{\xi}), \tag{3b}$$

collision step,

$$\frac{\partial h_2(\boldsymbol{X},\boldsymbol{\xi},t)}{\partial t}=Q(h_2(\boldsymbol{X},\boldsymbol{\zeta},t),h_2(\boldsymbol{X},\boldsymbol{\zeta},t))[\boldsymbol{\xi}],\quad 0<t\le\Delta t, \tag{4a}$$

$$h_2(\boldsymbol{X},\boldsymbol{\xi},0)=h_1(\boldsymbol{X},\boldsymbol{\xi},\Delta t), \tag{4b}$$

and the approximate solution of problem (1) at $t=\Delta t$ is obtained as $h_2(\boldsymbol{X},\boldsymbol{\xi},\Delta t)$.

Let us evaluate the truncation error of the approximate solution per time step Δt. In the following, we assume the smoothness of $f_0(\boldsymbol{X},\boldsymbol{\xi})$ for simplicity. The exact solution $f(\boldsymbol{X},\boldsymbol{\xi},\Delta t)$ and the approximate solution $h_2(\boldsymbol{X},\boldsymbol{\xi},\Delta t)$ are formally written as

$$f(\boldsymbol{X},\boldsymbol{\xi},\Delta t)=f_0(\boldsymbol{X}_0,\boldsymbol{\xi})+\int_0^{\Delta t}Q(f(\boldsymbol{X}[s],\boldsymbol{\zeta},s),\,f(\boldsymbol{X}[s],\boldsymbol{\zeta},s))[\boldsymbol{\xi}]\,ds, \tag{5}$$

$$h_2(\boldsymbol{X},\boldsymbol{\xi},\Delta t)=f_0(\boldsymbol{X}_0,\boldsymbol{\xi})+\int_0^{\Delta t}Q(h_2(\boldsymbol{X},\boldsymbol{\zeta},s),h_2(\boldsymbol{X},\boldsymbol{\zeta},s))[\boldsymbol{\xi}]\,ds, \tag{6}$$

where

$$\boldsymbol{X}[s]=\boldsymbol{X}-(\Delta t-s)\boldsymbol{\xi},\quad \boldsymbol{X}_0=\boldsymbol{X}[0]. \tag{7}$$

The difference between them is

$$\begin{aligned}f(\boldsymbol{X},\boldsymbol{\xi},\Delta t)-h_2(\boldsymbol{X},\boldsymbol{\xi},\Delta t)=\int_0^{\Delta t}\{&Q(f(\boldsymbol{X}[s],\boldsymbol{\zeta},s),\,f(\boldsymbol{X}[s],\boldsymbol{\zeta},s))[\boldsymbol{\xi}]\\&-Q(h_2(\boldsymbol{X},\boldsymbol{\zeta},s),h_2(\boldsymbol{X},\boldsymbol{\zeta},s))[\boldsymbol{\xi}]\}\,ds.\end{aligned} \tag{8}$$

Expanding $Q(f,\,f)$ in Eq. (8) around $s=0$, we have

$$\begin{aligned}Q(f(\boldsymbol{X}[s],\boldsymbol{\zeta},s),\,f(\boldsymbol{X}[s],\boldsymbol{\zeta},s))[\boldsymbol{\xi}]=&\,Q(f_0(\boldsymbol{X}_0,\boldsymbol{\zeta}),\,f_0(\boldsymbol{X}_0,\boldsymbol{\zeta}))[\boldsymbol{\xi}]\\&+2sQ\left(\left.\frac{df}{ds}\right|_{s=0},\,f_0(\boldsymbol{X}_0,\boldsymbol{\zeta})\right)[\boldsymbol{\xi}]+O(s^2),\end{aligned} \tag{9}$$

where

$$\begin{aligned}\left.\frac{df}{ds}\right|_{s=0}&=\left(\frac{\partial f}{\partial t}+\boldsymbol{\xi}\cdot\frac{\partial f}{\partial \boldsymbol{X}}\right)(\boldsymbol{X}_0,\boldsymbol{\zeta},0)\\&=(\boldsymbol{\xi}-\boldsymbol{\zeta})\frac{\partial f_0}{\partial \boldsymbol{X}}(\boldsymbol{X}_0,\boldsymbol{\zeta})+Q(f_0(\boldsymbol{X}_0,\boldsymbol{\zeta}),\,f_0(\boldsymbol{X}_0,\boldsymbol{\zeta}))[\boldsymbol{\xi}].\end{aligned} \tag{10}$$

Similarly,

$$\begin{aligned}Q(h_2(\boldsymbol{X},\boldsymbol{\zeta},s),h_2(\boldsymbol{X},\boldsymbol{\zeta},s))[\boldsymbol{\xi}]=&\,Q(h_2(\boldsymbol{X},\boldsymbol{\zeta},0),h_2(\boldsymbol{X},\boldsymbol{\zeta},0))[\boldsymbol{\xi}]\\&+2sQ\left(\frac{\partial h_2}{\partial t}(\boldsymbol{X},\boldsymbol{\zeta},0),h_2(\boldsymbol{X},\boldsymbol{\zeta},0)\right)[\boldsymbol{\xi}]+O(s^2).\end{aligned} \tag{11}$$

From Eq. (4a) and

$$\begin{aligned} h_2(\boldsymbol{X},\boldsymbol{\zeta},0) &= h_1(\boldsymbol{X},\boldsymbol{\zeta},\Delta t) \\ &= f_0(\boldsymbol{X}_0,\boldsymbol{\zeta}) + \Delta t(\boldsymbol{\xi}-\boldsymbol{\zeta})\frac{\partial f_0}{\partial \boldsymbol{X}}(\boldsymbol{X}_0,\boldsymbol{\zeta}) + O(\Delta t^2), \end{aligned} \tag{12}$$

we have

$$\begin{aligned} Q(h_2(\boldsymbol{X},\boldsymbol{\zeta},s), h_2(\boldsymbol{X},\boldsymbol{\zeta},s))[\boldsymbol{\xi}] = {} & Q(\,f_0(\boldsymbol{X}_0,\boldsymbol{\zeta}),\ f_0(\boldsymbol{X}_0,\boldsymbol{\zeta}))[\boldsymbol{\xi}] \\ & + 2\Delta t\, Q\left((\boldsymbol{\xi}-\boldsymbol{\zeta})\frac{\partial f_0}{\partial \boldsymbol{X}}(\boldsymbol{X}_0,\boldsymbol{\zeta}),\ f_0(\boldsymbol{X}_0,\boldsymbol{\zeta})\right)[\boldsymbol{\xi}] \\ & + 2s\, Q(Q(\,f_0(\boldsymbol{X}_0,\boldsymbol{\eta}),\ f_0(\boldsymbol{X}_0,\boldsymbol{\eta}))[\boldsymbol{\zeta}],\ f_0(\boldsymbol{X}_0,\boldsymbol{\zeta}))[\boldsymbol{\xi}] \\ & + O(s^2) + O(s\Delta t) + O(\Delta t^2). \end{aligned} \tag{13}$$

From Eqs. (9), (10), and (13), we obtain

$$f(\boldsymbol{X},\boldsymbol{\xi},\Delta t) - h_2(\boldsymbol{X},\boldsymbol{\xi},\Delta t) = -\Delta t^2 Q\left((\boldsymbol{\xi}-\boldsymbol{\zeta})\frac{\partial f_0}{\partial \boldsymbol{X}}(\boldsymbol{X}_0,\boldsymbol{\zeta}),\ f_0(\boldsymbol{X}_0,\boldsymbol{\zeta})\right)[\boldsymbol{\xi}] + O(\Delta t^3). \tag{14}$$

Thus, it is concluded that the truncation error of the splitting method is not $O(\Delta t^3)$ but $O(\Delta t^2)$. In view of the accumulation of the error, we find that the splitting method is at most first-order accurate in Δt.

The above estimate is contrary to Bogomolov's result [4]. He evaluated the collision integrals in Eq. (8) but confused $\boldsymbol{\zeta}$ and $\boldsymbol{\xi}$, unfortunately. This miscalculation led the above-mentioned misunderstanding. In the splitting method, the collision step may also be performed before the convection step. In this case, the leading term of the truncation error differs only in the sign from that shown in Eq. (14).

III. HIGHER ORDER TIME DIFFERENCING METHOD

As a by-product of the discussion in Section II (Eqs. (5), (9), and (10)), we obtain a second-order accurate formula:

$$\begin{aligned} h_1(\boldsymbol{X},\boldsymbol{\xi}) = {} & f_0(\boldsymbol{X},\boldsymbol{\xi}) + \Delta t\, Q(\,f_0(\boldsymbol{X},\boldsymbol{\zeta}),\ f_0(\boldsymbol{X},\boldsymbol{\zeta}))[\boldsymbol{\xi}] \\ & + \Delta t^2\Bigg\{ Q(Q(\,f_0(\boldsymbol{X},\boldsymbol{\eta}),\ f_0(\boldsymbol{X},\boldsymbol{\eta}))[\boldsymbol{\zeta}],\ f_0(\boldsymbol{X},\boldsymbol{\zeta}))[\boldsymbol{\xi}] \\ & + \sum_{i=1}^{3}\xi_i\, Q\left(\frac{\partial f_0(\boldsymbol{X},\boldsymbol{\zeta})}{\partial X_i},\ f_0(\boldsymbol{X},\boldsymbol{\zeta})\right)[\boldsymbol{\xi}] \\ & - Q\left(\boldsymbol{\zeta}\cdot\frac{\partial f_0(\boldsymbol{X},\boldsymbol{\zeta})}{\partial \boldsymbol{X}},\ f_0(\boldsymbol{X},\boldsymbol{\zeta})\right)[\boldsymbol{\xi}]\Bigg\}, \end{aligned} \tag{15a}$$

$$f(\boldsymbol{X},\boldsymbol{\xi},\Delta t) = h_1(\boldsymbol{X}_0,\boldsymbol{\xi}). \tag{15b}$$

The term multiplied by Δt^2 is the correction to the conventional splitting method. Without

the space derivatives of f_0, Eq. (15) corresponds to the splitting formula with second-order accurate time-integration in the collision step. Because of the collision integrals multiplied by ξ_i, only the conservation of mass is satisfied in Eq. (15a). A second-order accurate formula which is conservative with respect to mass, momenta, and energy will be shown later.

Let $\boldsymbol{X}^{(i)}$ and $\boldsymbol{\xi}^{(j)}$ be the grids in $\boldsymbol{X}$ space and in $\boldsymbol{\xi}$ space, respectively. The discrete ordinates approximation of the above formula is a desired numerical method, which consists of two steps:

(i) Compute $\partial f_0(\boldsymbol{X}^{(i)}, \boldsymbol{\xi}^{(k)})/\partial \boldsymbol{X}$ from the values of f_0 on some grids around $\boldsymbol{X}^{(i)}$ using a suitable finite difference formula and compute $h_1(\boldsymbol{X}^{(i)}, \boldsymbol{\xi}^{(j)})$ from $f_0(\boldsymbol{X}^{(i)}, \boldsymbol{\xi}^{(k)})$ and $\partial f_0(\boldsymbol{X}^{(i)}, \boldsymbol{\xi}^{(k)})/\partial \boldsymbol{X}$ according to Eq. (15a). Several methods have been proposed for the computation of the collision integral of the full (or model) Boltzmann equation. We refer the reader to Refs. [6–9] and omit the details here.

(ii) Compute the nearest grid from $\boldsymbol{X}_0^{(i,j)} (\equiv \boldsymbol{X}^{(i)} - \Delta t \boldsymbol{\xi}^{(j)})$ and let it be $\boldsymbol{X}^{P(i,j)}$. Compute $h_1(\boldsymbol{X}^{(i,j)}, \boldsymbol{\xi}^{(j)})$ from the values of h_1 on some grids around $\boldsymbol{X}^{P(i,j)}$ using a suitable interpolation formula.

Step (i) and step (ii) correspond to the collision step and the convection step in the splitting method, respectively. We can also compute the convection step first. In this case, Eq. (15b) is replaced by $h_1(\boldsymbol{X}, \boldsymbol{\xi}) = f_0(\boldsymbol{X}_0, \boldsymbol{\xi})$ and h_1 and f_0 in Eq. (15a) by $f(\boldsymbol{X}, \boldsymbol{\xi}, \Delta t)$ and h_1, respectively.

The accuracy in each step which is necessary for the second-order accuracy of total computation is as follows. In contrast to the case of the conventional splitting method, the error of computation of the collision integral should be at most $O(\Delta t^2)$, which seems to become a severe condition for some of the above-cited methods in the actual computation. The accuracy data presented in Ref. [8], however, indicate that such accuracy can be achieved at least for the case where the distribution function is axially symmetric in the velocity space. The truncation error of the interpolation in step (ii) should be at most $O(\Delta t^3)$ [and that of $\partial f_0/\partial \boldsymbol{X}$ should be at most $O(\Delta t)$]. Thus, the interpolation formula should be higher-order accurate.

As for the convection step, the interpolation around $\boldsymbol{X}^{P(i,j)}$ is always used and the extrapolation, which causes the instability, is never used. This enables the use of a time step larger than the value restricted by the Courant–Friedlichs–Lewy (CFL) condition. This does not guarantee the stability of total computation, however. Since the collision term is not always positive, the numerical solution begins to take negative and appreciable values on some grids for a large Δt. This causes the instability. The computation is, however, stable while the magnitude of the negative value is negligibly small.

In the above approximation formula for Eq. (5), the integrand is replaced by the first two terms of its expansion around $s = 0$. If the value of the integrand at $s = \Delta t$ is known *a priori*, the integral can be computed by the trapezoidal rule without loss of the higher order accuracy, since the truncation error of this rule is $O(\Delta t^3)$. In the case where the collision term is linear with respect to f, we can obtain the solution, f at $s = \Delta t$, using this rule without the value of the integrand at $s = \Delta t$. That is, the discrete ordinates approximation of the linear (or linearized) collision term is expressed as the product of the numerical kernel matrix $\boldsymbol{W}$ and the vector corresponding to the distribution function f (see, e.g., Ref. [10]) and the computation is reduced to the inversion of $\boldsymbol{I} - (\Delta t/2)\boldsymbol{W}$, where $\boldsymbol{I}$ is the unit matrix. This technique has been developed by Demeio [11] in the analysis of the one-dimensional

Vlasov–Poisson equation with BGK-like collision term, where the temperature and velocity in the local Maxwellian and the collision frequency are constant. In the nonlinear case, however, the inversion of the collision term is not a good idea. Fortunately, a simpler way, which is applicable to the nonlinear case, is available. That is, the integrand at $s = \Delta t$ may be computed from the value of f obtained by the conventional splitting method. The corresponding formula is

$$f(\boldsymbol{X}, \boldsymbol{\xi}, \Delta t) = f_0(\boldsymbol{X}_0, \boldsymbol{\xi}) + \frac{\Delta t}{2}\{Q(f_1(\boldsymbol{X}, \zeta), f_1(\boldsymbol{X}, \zeta))[\boldsymbol{\xi}] + Q(f_0(\boldsymbol{X}_0, \zeta), f_0(\boldsymbol{X}_0, \zeta))[\boldsymbol{\xi}]\}, \tag{16a}$$

$$f_1(\boldsymbol{X}, \boldsymbol{\xi}) = f_0(\boldsymbol{X}_0, \boldsymbol{\xi}) + \Delta t\, Q(f_0(\boldsymbol{X}_0, \zeta), f_0(\boldsymbol{X}_0, \zeta))[\boldsymbol{\xi}]. \tag{16b}$$

The truncation error of the above formula is also $O(\Delta t^3)$, since $f_1(\boldsymbol{X}, \boldsymbol{\xi}) - f(\boldsymbol{X}, \boldsymbol{\xi}, \Delta t) = O(\Delta t^2)$. Noting that

$$f_1(\boldsymbol{X}, \zeta) = f_0(\boldsymbol{X}_0, \zeta) + \Delta t(\boldsymbol{\xi} - \zeta)\frac{\partial f_0}{\partial \boldsymbol{X}}(\boldsymbol{X}_0, \zeta) + \Delta t\, Q(f_0(\boldsymbol{X}_0, \eta), f_0(\boldsymbol{X}_0, \eta))[\zeta] + O(\Delta t^2), \tag{17}$$

we find that the former formula (15) is derived from the latter (16). By rewriting formula (16) in the form

$$f(\boldsymbol{X}, \boldsymbol{\xi}, \Delta t) = h(\boldsymbol{X}_0, \boldsymbol{\xi}) + \frac{\Delta t}{2} Q(f_1(\boldsymbol{X}, \zeta), f_1(\boldsymbol{X}, \zeta))[\boldsymbol{\xi}], \tag{18a}$$

$$h(\boldsymbol{X}, \boldsymbol{\xi}) = f_0(\boldsymbol{X}, \boldsymbol{\xi}) + \frac{\Delta t}{2} Q(f_0(\boldsymbol{X}, \zeta), f_0(\boldsymbol{X}, \zeta))[\boldsymbol{\xi}], \tag{18b}$$

we find that this formula is conservative; the translation and the collision integrals do not contribute to the variation of the total mass, momenta, and energy. Incidentally, there is no differential term in the formula (16), which is advantageous for the extension to the stochastic approach (see Section V). The computation for Eq. (16) is simpler than that for Eq. (15) and is omitted here.

We derived two higher order differencing methods for the full Boltzmann equation. These methods are summarized as higher order integration formulas for the integral of the collision term along the characteristic line. Formula (16) is one of the simplest examples; the derivation is simple and the truncation error is easily estimated. Of course, there are other higher order schemes for the Boltzmann equation. For example, the application of Strang's splitting method [12] is one of them. Strang's splitting method for the Boltzmann equation consists of the convection step for $\Delta t/2$, the collision step for Δt, and the convection step for $\Delta t/2$; the collision step is computed between two convection steps. The error analysis, similar to that in Section II, shows that the second-order accuracy can be realized by using this formulation. This is easily seen from the last sentence in Section II; Strang's splitting method is regarded as the combination of two conventional splitting methods of different order, i.e., convection + collision and collision + convection, and the leading errors of these two methods are canceled. Since the accuracy of the collision step required in Strang's splitting method is at least second order, we have to compute the collision

integral twice, which means that the amount of computation is almost the same as that for formula (16).

IV. NUMERICAL DEMONSTRATION OF HIGHER ORDER ACCURACY

In this section, we demonstrate the accuracy of higher-order time differencing methods developed in Section III (Eqs. (15) and (16)) numerically in the problem of the propagation of a normal shock wave. We consider the case where the shock front is propagating into a gas at rest with the velocity in the X_1 direction. We use the BGK model equation as the basic equation for simplicity; the collision term of the BGK model equation can be computed accurately without any difficulty in the present one-dimensional case. The explanation of the present method for the one-dimensional BGK model equation is given in the Appendix.

We first computed a stationary shock for $M = 2$, where M is the upstream Mach number, using the present method (Eq. (15)), and we obtained the initial value of the time-dependent problem by applying Galilei transformation to the stationary shock solution.

Before proceeding to the explanation of the propagation problem, we summarize the notations: $X_1 = 2^{-1}\sqrt{\pi} l_* \tilde{x}$ is the space coordinate; $t = \sqrt{\pi} l_* (8RT_*)^{-1/2} \tilde{t}$ is the time; $(2RT_*)^{-1/2}\tilde{\xi}_i$ is the molecular velocity; and $\rho_* (2\pi RT_*)^{-3/2} \tilde{f}(\tilde{x}, \tilde{\xi}_i, \tilde{t})$ is the distribution function of gas molecules, where l_* is the mean free path of the gas molecules at the front side equilibrium state at rest at temperature T_*, density ρ_*, and R is the specific gas constant; $\rho_* \tilde{\rho}$, $(2RT_*)^{1/2}\tilde{v}_i$ $[\tilde{v}_i = (\tilde{v}, 0, 0)]$, $T_* \tilde{T}$ are the density, flow velocity, and temperature of the gas, respectively (see the Appendix for the definitions of $\tilde{\rho}$, $\tilde{v}$, and $\tilde{T}$).

The grid systems used in the propagation problem are as follows. The space region is limited to $-40 \le \tilde{x} \le 40$ and is divided into 400 uniform sections; the width $\Delta\tilde{x}$ is 0.2. The region for $\tilde{\xi}_1$ is limited to $-5.675 \lesssim \tilde{\xi}_1 \lesssim 9.325$ (see the Appendix, where the components $\tilde{\xi}_2$ and $\tilde{\xi}_3$ are eliminated by using Chu's method [13]) and is divided into 100 uniform sections.

The shock wave was located around $\tilde{x} = 0$ at $\tilde{t} = 0$ and the computation was carried out until $\tilde{t} = 4$ for four cases of the time step $\Delta\tilde{t}$; $\Delta\tilde{t}$ in case n ($n = 0, 1, 2, 3$) is $0.4/2^n$; i.e. $\Delta\tilde{t} = 0.4, 0.2, 0.1$, and 0.05. It was confirmed the the disturbance at the numerical boundary $\tilde{x} = \pm 40$ was negligibly small during the computation; the position of the average density $[\tilde{\rho}(\tilde{x} = -\infty) + \tilde{\rho}(\tilde{x} = \infty)]/2$ was $\tilde{x} \simeq -0.61$ at $\tilde{t} = 0$ and $\tilde{x} \simeq 6.69$ at $\tilde{t} = 4$ (the thickness of the shock wave is $O(1)$). As noted in Section III, the truncation error of the interpolation should be at most $O(\Delta\tilde{t}^3)$. The truncation error of the interpolation formula used in the present computation is $O(\Delta\tilde{x}^7)$ (see the Appendix) and $\Delta\tilde{x}^7 < \Delta\tilde{t}^3$ for all cases of the time step. It should be noted that the CFL condition is not satisfied for all cases of the time step (see the fifth paragraph in Section III).

The macroscopic variable for case n, $H^n (= \tilde{\rho}^n, \tilde{v}^n, \tilde{T}^n)$, was compared with that for case $n + 1$. The spatial average of the difference between H^n and H^{n+1},

$$\bar{H}^n(\tilde{t}) = \frac{\sum_{i=1}^{N_p} \left| H^n\left(\tilde{x}^{(i)}, \tilde{t}\right) - H^{n+1}\left(\tilde{x}^{(i)}, \tilde{t}\right) \right|}{N_p}, \tag{19}$$

where $\tilde{x}^{(i)} (i = 1, \ldots, N_p (= 401))$ are $\tilde{x}$ grids, is approximately proportional to $4^{-n} (\sim \Delta\tilde{t}^2)$ for all times which are common for all cases of the time step. The $\bar{\rho}^n$, $\bar{v}^n$, and $\bar{T}^n$ at $\tilde{t} = 4$ are tabulated in Table 1. From the conservation law in a coordinate system moving with the

TABLE 1
The Difference between Case n and Case $n+1$ at $\tilde{t}=4$

	$\overline{\rho}^0$ ($\Delta\tilde{t}=0.4, 0.2$)	$\overline{\rho}^1$ ($\Delta\tilde{t}=0.2, 0.1$)	$\overline{\rho}^2$ ($\Delta\tilde{t}=0.1, 0.05$)
Eq. (15)	4.7×10^{-4}	8.2×10^{-5}	1.7×10^{-5}
Eq. (16)	3.1×10^{-4}	6.2×10^{-5}	1.3×10^{-5}
Modified Euler	1.3×10^{-3}	1.7×10^{-4}	3.6×10^{-5}
Conventional	2.9×10^{-3}	1.3×10^{-3}	6.1×10^{-4}
	$\overline{v}^0$ ($\Delta\tilde{t}=0.4, 0.2$)	$\overline{v}^1$ ($\Delta\tilde{t}=0.2, 0.1$)	$\overline{v}^2$ ($\Delta\tilde{t}=0.1, 0.05$)
Eq. (15)	3.7×10^{-4}	7.1×10^{-5}	1.5×10^{-5}
Eq. (16)	1.7×10^{-4}	3.9×10^{-5}	8.3×10^{-6}
Modified Euler	1.2×10^{-3}	2.0×10^{-4}	4.1×10^{-5}
Conventional	2.1×10^{-3}	9.9×10^{-4}	4.8×10^{-4}
	$\overline{T}^0$ ($\Delta\tilde{t}=0.4, 0.2$)	$\overline{T}^1$ ($\Delta\tilde{t}=0.2, 0.1$)	$\overline{T}^2$ ($\Delta\tilde{t}=0.1, 0.05$)
Eq. (15)	5.8×10^{-4}	1.1×10^{-4}	2.4×10^{-5}
Eq. (16)	2.2×10^{-4}	5.3×10^{-5}	1.3×10^{-5}
Modified Euler	1.8×10^{-3}	3.1×10^{-4}	6.9×10^{-5}
Conventional	3.2×10^{-3}	1.5×10^{-3}	7.4×10^{-4}

shock front velocity $(U,0,0)$, where $U=\sqrt{5/6}M$, the moments of the present unsteady solution,

$$K(\tilde{x},\tilde{t})=\pi^{-3/2}\int(\tilde{\xi}_1-U)\tilde{f}(\tilde{x},\tilde{t})d\tilde{\boldsymbol{\xi}}, \tag{20a}$$

$$L(\tilde{x},\tilde{t})=\pi^{-3/2}\int(\tilde{\xi}_1-U)^2\tilde{f}(\tilde{x},\tilde{t})d\tilde{\boldsymbol{\xi}}, \tag{20b}$$

$$Z(\tilde{x},\tilde{t})=\pi^{-3/2}\int(\tilde{\xi}_1-U)\left[(\tilde{\xi}_1-U)^2+\tilde{\xi}_2^2+\tilde{\xi}_3^2\right]\tilde{f}(\tilde{x},\tilde{t})d\tilde{\boldsymbol{\xi}}, \tag{20c}$$

should be $-U$, $1/2+U^2$, and $-5U/2-U^3$, respectively. As the measure of deviation from the exact solution, we examine

$$\overline{K}^n(\tilde{t})=\frac{\sum_{i=1}^{N_p}\left|K^n\left(\tilde{x}^{(i)},\tilde{t}\right)+U\right|}{N_p}, \tag{21a}$$

$$\overline{L}^n(\tilde{t})=\frac{\sum_{i=1}^{N_p}\left|L^n\left(\tilde{x}^{(i)},\tilde{t}\right)-\frac{1}{2}-U^2\right|}{N_p}, \tag{21b}$$

$$\overline{Z}^n(\tilde{t})=\frac{\sum_{i=1}^{N_p}\left|Z^n\left(\tilde{x}^{(i)},\tilde{t}\right)+\frac{5U}{2}+U^3\right|}{N_p}, \tag{21c}$$

where the superscript n denotes the case. The averaged deviations $\overline{K}^n$, $\overline{L}^n$, and $\overline{Z}^n$ are approximately proportional to $4^{-n}\sim\Delta\tilde{t}^2$ for all common times. The $\overline{K}^n$, $\overline{L}^n$, and $\overline{Z}^n$ ($n=0,1,2,3$) at $\tilde{t}=4$ are tabulated in Table 2. These tables indicate that the higher order accuracy is realized by using present methods. If the space derivatives $\partial f_0/\partial X_i$ are omitted in Eq. (15), the resulting formula corresponds to the splitting method with the time integration by the modified Euler method. The formula without the terms multiplied

TABLE 2
The Deviation from the Exact Value at $\tilde{t} = 4$

	$\bar{K}^0$ ($\Delta\tilde{t} = 0.4$)	$\bar{K}^1$ ($\Delta\tilde{t} = 0.2$)	$\bar{K}^2$ ($\Delta\tilde{t} = 0.1$)	$\bar{K}^3$ ($\Delta\tilde{t} = 0.05$)
Eq. (15)	5.6×10^{-4}	1.3×10^{-4}	3.1×10^{-5}	7.3×10^{-6}
Eq. (16)	2.4×10^{-4}	6.1×10^{-5}	1.6×10^{-5}	4.3×10^{-6}
Modified Euler	1.6×10^{-3}	3.9×10^{-4}	1.6×10^{-4}	7.8×10^{-5}
Conventional	3.7×10^{-3}	1.8×10^{-3}	9.1×10^{-4}	4.6×10^{-4}
	$\bar{L}^0$ ($\Delta\tilde{t} = 0.4$)	$\bar{L}^1$ ($\Delta\tilde{t} = 0.2$)	$\bar{L}^2$ ($\Delta\tilde{t} = 0.1$)	$\bar{L}^3$ ($\Delta\tilde{t} = 0.05$)
Eq. (15)	1.1×10^{-3}	2.7×10^{-4}	6.5×10^{-5}	1.6×10^{-5}
Eq. (16)	7.6×10^{-4}	1.5×10^{-4}	3.6×10^{-5}	9.1×10^{-6}
Modified Euler	6.9×10^{-3}	3.1×10^{-3}	1.5×10^{-3}	7.7×10^{-4}
Conventional	8.3×10^{-3}	4.1×10^{-3}	2.0×10^{-3}	1.0×10^{-3}
	$\bar{Z}^0$ ($\Delta\tilde{t} = 0.4$)	$\bar{Z}^1$ ($\Delta\tilde{t} = 0.2$)	$\bar{Z}^2$ ($\Delta\tilde{t} = 0.1$)	$\bar{Z}^3$ ($\Delta\tilde{t} = 0.05$)
Eq. (15)	3.4×10^{-3}	7.8×10^{-4}	1.9×10^{-4}	4.5×10^{-5}
Eq. (16)	1.2×10^{-3}	2.8×10^{-4}	7.2×10^{-5}	2.0×10^{-5}
Modified Euler	6.5×10^{-3}	2.1×10^{-3}	1.1×10^{-3}	5.7×10^{-4}
Conventional	1.5×10^{-2}	7.5×10^{-3}	3.8×10^{-3}	1.9×10^{-3}

by Δt^2 corresponds to the conventional splitting method. In these tables, the data obtained by these formulas for the BGK model equation are also tabulated for comparison. The data obtained by the conventional splitting method are approximately proportional to $\Delta\tilde{t}$; the accuracy of the conventional splitting method is first order. Although the accuracy is improved by using the modified Euler method in the collision step (see Table 1), the deviation from the exact solution is proportional to Δt (see Table 2), and thus, the accuracy is still first order. Finally, we remark that the higher order accuracy is realized by the nonconservative formula (15), as well as the conservative formula. This shows that the conservative property of the scheme is not the necessary condition for the convergence of the numerical solution.

V. IMPROVEMENT OF DSMC PROCEDURE

In this section, we propose a way to extend the higher-order deterministic method (16) to the stochastic approach. We first rewrite Eq. (16) in the form

$$f(\boldsymbol{X}, \boldsymbol{\xi}, \Delta t) = \frac{f_0(\boldsymbol{X}_0, \boldsymbol{\xi})}{2} + \frac{f_1(\boldsymbol{X}, \boldsymbol{\xi})}{2} + 2\Delta t\, Q\left(\frac{f_1(\boldsymbol{X}, \zeta)}{2}, \frac{f_1(\boldsymbol{X}, \zeta)}{2}\right)[\boldsymbol{\xi}], \quad (22a)$$

$$\frac{f_1(\boldsymbol{X}, \boldsymbol{\xi})}{2} = \frac{f_0(\boldsymbol{X}_0, \boldsymbol{\xi})}{2} + 2\Delta t\, Q\left(\frac{f_0(\boldsymbol{X}_0, \zeta)}{2}, \frac{f_0(\boldsymbol{X}_0, \zeta)}{2}\right)[\boldsymbol{\xi}]. \quad (22b)$$

In view of the formula which corresponds to the conventional DSMC method, i.e.

$$f(\boldsymbol{X}, \boldsymbol{\xi}, \Delta t) = f_0(\boldsymbol{X}_0, \boldsymbol{\xi}) + \Delta t\, Q(f_0(\boldsymbol{X}_0, \zeta),\ f_0(\boldsymbol{X}_0, \zeta))[\boldsymbol{\xi}], \quad (23)$$

formula (22) is interpreted as the following simulation procedure:

(i) Perform the convection step (free molecular flow) for the time step Δt.
(ii) For each cell, perform the steps (a), (b), (c) below.

(a) Choose $[N_c/2]$ particles randomly, where N_c is the number of particles in a cell and [ ] denotes the greatest integer function.

(b) For the particles chosen in step (a), perform the collision step for time step $2\Delta t$ (the probability of collision is doubled).

(c) Repeat step (b) again.

In step (i), which is the same as the convection step in the conventional DSMC method, $f_0(\boldsymbol{X}_0, \boldsymbol{\xi})$ is produced. In the step (ii.a) the particles are divided into two groups, each of which represents $f_0(\boldsymbol{X}_0, \boldsymbol{\xi})/2$. The particles which are not chosen in step (ii.a) represent the first term on the right-hand side of Eq. (22a). The particles chosen in step (ii.a) represent $f_1(\boldsymbol{X}, \boldsymbol{\xi})/2$ after step (ii.b) and the sum of the second and third terms on the right-hand side of Eq. (22a) after step (ii.c). Step (ii) is one of the second-order accurate methods for the spatially homogeneous Boltzmann equation. This step is related to Eq. (22). Higher order accuracy of the total computation is not guaranteed if this step is replaced by other second-order methods.

In the conventional DSMC method, the particles may collide more than once during the time step Δt. The influence of recollision is of the order of Δt^2, which is of negligible order in Eq. (23). In the present simulation procedure, however, the recollision is not allowed in each step, (ii.b) and (ii.c) (the particles which collide in step (ii.b) may collide again in step (ii.c)). Since the present simulation method is based on the formula (22), which is correct up to $O(\Delta t^2)$, the influence of the recollision is no longer negligible. In order to confirm the necessity of this restriction, we carried out the preliminary DSMC computation for a spatially homogeneous unsteady problem (the molecular model is a hard sphere and the initial condition is $\tilde{f} = \exp(-\tilde{\xi}_1^2/3 - \tilde{\xi}_2^2 - \tilde{\xi}_3^2)$; cf. Section IV for the notation). It was observed that the permission of the recollision spoiled the second-order accuracy. This is in contrast to the conventional DSMC procedure. In this case, as is mentioned in Ref. [2] and was also observed in the above preliminary computation, the permission of recollision improves the accuracy of the collision step, although, to the author's knowledge, it has not yet been made legitimate mathematically. As shown in Section II and demonstrated in Section IV, however, the improvement for the spatially homogeneous equation is not sufficient for higher order accuracy in the spatially nonhomogeneous case, where the present simulation procedure is expected to work. Another improved DSMC procedure is obtained by applying Strang's splitting method. As noted in Section III, the collision step in Strang's splitting method must be at least second-order accurate. In this case, the collision step can be computed by using other second-order methods. If the collision step of the conventional DSMC method, which permits the recollision, were shown to be second-order accurate, then the simplest higher order procedure would be the Strang-type procedure.

In most cases of unsteady problems, the final result of the DSMC method is obtained as the ensemble average. The present simulation procedure becomes meaningless unless the error due to the ensemble average is at most of the order of Δt^2. In the above preliminary numerical experiment, the computation was carried out for $(N_c, N_s) = (100, 1000000)$, $(10000, 10000)$, $(1000000, 100)$, where N_c is the number of particles used in the simulation and N_s is that of samples used in the ensemble average. As for the values of the moments $\pi^{-3/2} \int \tilde{\xi}_i^2 \tilde{f} d\tilde{\boldsymbol{\xi}}$ $(i = 1, 2, 3)$, which are $O(1)$, the difference between the first and second cases appears at the third figure and that between the second and the third cases at the fourth figure. Judging from this, a large number of particles are necessary for the meaningful use of the present simulation procedure. Such a computation, however, is not beyond

the ability of the presently available computers, at least for the spatially one-dimensional case.

VI. CONCLUDING REMARKS

The conventional splitting method for the Boltzmann equation is derived as the first-order approximation of the integral form of the equation along its characteristic line. Higher order accuracy is never realized by any improvements in the framework of the first-order approximation. In the present study, the above statement is confirmed and the higher order time differencing methods for the full Boltzmann equation are constructed as the second-order approximation of the integral form. The accuracy of higher order methods is demonstrated numerically for the BGK model equation. The extension to the stochastic method is also proposed, together with some remarks. The numerical analyses based on the full Boltzmann equation using the present higher order approximation method and the validation of the improved DSMC method in spatially nonhomogeneous problems are in preparation.

APPENDIX: APPLICATION TO ONE-DIMENSIONAL BGK EQUATION

The BGK model equation in the present one-dimensional case is written as

$$\frac{\partial f}{\partial t} + \xi_1 \frac{\partial f}{\partial X_1} = A_c \rho (f_e - f), \tag{A1}$$

$$f_e = \frac{\rho}{(2\pi RT)^{3/2}} \exp\left(- \frac{(\xi_1 - v)^2 + \xi_2^2 + \xi_3^3}{2RT} \right), \tag{A2}$$

$$\rho = \int f d\boldsymbol{\xi},$$

$$v = \int \xi_1 f d\boldsymbol{\xi}, \tag{A3}$$

$$T = \frac{1}{3R\rho} \int \left[(\xi_1 - \rho v)^2 + \xi_2^2 + \xi_3^2 \right] f d\boldsymbol{\xi},$$

where ρ is the gas density, $v_i = (v, 0, 0)$ is the gas flow velocity, T is the gas temperature, R is the specific gas constant, and A_c is a constant ($A_c \rho$ is the collision frequency of gas molecules). The domain of integration in Eq. (A3) is the whole velocity space.

According to Chu [13], the molecular velocity components ξ_2 and ξ_3 can be eliminated in the present one-dimensional case. Multiplying Eq. (A1) by 1 and $\xi_2^2 + \xi_3^2$ and integrating the results over the whole $\xi_2 \xi_3$ plane, we have

$$\frac{\partial \boldsymbol{\Phi}}{\partial \tilde{t}} + \tilde{\xi} \frac{\partial \boldsymbol{\Phi}}{\partial \tilde{x}} = \tilde{\rho} (\boldsymbol{\Phi}_e - \boldsymbol{\Phi}), \tag{A4a}$$

$$\boldsymbol{\Phi} = \begin{pmatrix} g_+ \\ g_- \end{pmatrix}, \tag{A4b}$$

$$\boldsymbol{\Phi}_e = \begin{pmatrix} g_{e+} \\ g_{e-} \end{pmatrix} = \frac{\pi \tilde{\rho}}{\tilde{T}^{1/2}} \begin{pmatrix} 1 \\ \tilde{T} \end{pmatrix} \exp\left(- \frac{(\tilde{\xi} - \tilde{v})^2}{\tilde{T}} \right), \tag{A4c}$$

$$\tilde{\rho} = \frac{1}{\pi^{3/2}} \int_{-\infty}^{\infty} g_+ d\tilde{\xi},$$
$$\tilde{v} = \frac{1}{\pi^{3/2}\tilde{\rho}} \int_{-\infty}^{\infty} \tilde{\xi} g_+ d\tilde{\xi}, \tag{A4d}$$
$$\tilde{T} = \frac{2}{3\pi^{3/2}\tilde{\rho}} \left(\int_{-\infty}^{\infty} (\tilde{\xi} - \tilde{v})^2 g_+ d\tilde{\xi} + \int_{-\infty}^{\infty} g_- d\tilde{\xi} \right),$$

where

$$g_+ = \pi^{3/2} (2RT_*)^{1/2} \rho_*^{-1} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f d\xi_2 d\xi_3, \tag{A5a}$$

$$g_- = \pi^{3/2} (2RT_*)^{-1/2} \rho_*^{-1} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left(\xi_2^2 + \xi_3^2\right) f d\xi_2 d\xi_3, \tag{A5b}$$

$$\tilde{x} = 2\pi^{-1/2} l_*^{-1} X_1, \quad \tilde{t} = (8RT_*/\pi)^{1/2} l_*^{-1} t,$$
$$\tilde{\xi} = (2RT_*)^{-1/2} \xi_1, \quad \tilde{\rho} = \rho_*^{-1} \rho, \tag{A6}$$
$$\tilde{v} = (2RT_*)^{1/2} v, \quad \tilde{T} = T_*^{-1} T,$$

and $l_*[= (8RT_*/\pi)^{1/2} (A_c \rho_*)^{-1}]$ is the mean free path of the gas molecules at the equilibrium state at rest at the temperature T_* and density p_*.

In Section III, we presented two formulas for the full Boltzmann equation (Eqs. (15) and (16)). Since the formula which corresponds to Eq. (16) is simpler than that which corresponds to Eq. (15), we omit the former and show only the latter. The formula corresponding to (15) is

$$\boldsymbol{h}_1(\tilde{x}, \tilde{\xi}) = \boldsymbol{\Phi}(\tilde{x}, \tilde{\xi}, 0) + \Delta\tilde{t} \boldsymbol{C}(\tilde{x}, \tilde{\xi}, 0) + \frac{\Delta\tilde{t}^2}{2} \left(\frac{\partial \boldsymbol{C}(\tilde{x}, \tilde{\xi}, 0)}{\partial \tilde{t}} + \tilde{\xi} \frac{\partial \boldsymbol{C}(\tilde{x}, \tilde{\xi}, 0)}{\partial \tilde{x}} \right), \tag{A7a}$$

$$\boldsymbol{\Phi}(\tilde{x}, \tilde{\xi}, \Delta\tilde{t}) = \boldsymbol{h}_1(\tilde{x}_0, \tilde{\xi}), \tag{A7b}$$

where

$$\boldsymbol{C} = \tilde{\rho}(\boldsymbol{\Phi}_e - \boldsymbol{\Phi}), \tag{A8a}$$
$$\tilde{x}_0 = \tilde{x} - \Delta\tilde{t}\tilde{\xi}. \tag{A8b}$$

The time derivatives in Eq. (A7a) are evaluated as follows. From Eq. (A4a), we have

$$\left(\frac{\partial}{\partial \tilde{t}} + \tilde{\xi} \frac{\partial}{\partial \tilde{x}} \right) \boldsymbol{C} = (\boldsymbol{\Phi}_e - \boldsymbol{\Phi}) \left(\frac{\partial \tilde{\rho}}{\partial \tilde{t}} + \tilde{\xi} \frac{\partial \tilde{\rho}}{\partial \tilde{x}} - \tilde{\rho}^2 \right) + \tilde{\rho} \left(\frac{\partial}{\partial \tilde{t}} + \tilde{\xi} \frac{\partial}{\partial \tilde{x}} \right) \boldsymbol{\Phi}_e, \tag{A9}$$

$$\tilde{\rho} \frac{\partial g_{e\pm}}{\partial \alpha} = g_{e\pm} \left[\frac{\partial \tilde{\rho}}{\partial \alpha} + \frac{2(\tilde{\xi} - \tilde{v})\tilde{\rho}}{\tilde{T}} \frac{\partial \tilde{v}}{\partial \alpha} - \left(\pm \frac{1}{2\tilde{T}} - \frac{(\tilde{\xi} - \tilde{v})^2}{\tilde{T}^2} \right) \tilde{\rho} \frac{\partial \tilde{T}}{\partial \alpha} \right]$$
$$(\alpha = \tilde{t}, \tilde{x}), \tag{A10}$$

where the time derivatives of the macroscopic varibles are given by

$$\frac{\partial \tilde{\rho}}{\partial \tilde{t}} = -\frac{\partial \tilde{M}_+^1}{\partial \tilde{x}}, \tag{A11a}$$

$$\tilde{\rho}\frac{\partial \tilde{v}}{\partial \tilde{t}} = \tilde{v}\frac{\partial \tilde{M}_+^1}{\partial \tilde{x}} - \frac{\partial \tilde{M}_+^2}{\partial \tilde{x}}, \tag{A11b}$$

$$\tilde{\rho}\frac{\partial \tilde{T}}{\partial \tilde{t}} = -\frac{2}{3}\frac{\partial(\tilde{M}_+^3 + \tilde{M}_-^1)}{\partial \tilde{x}} + \frac{4}{3}\tilde{v}\frac{\partial \tilde{M}_+^2}{\partial \tilde{x}} + \left(\tilde{T} - \frac{2}{3}\tilde{v}^2\right)\frac{\partial \tilde{M}_+^1}{\partial \tilde{x}}, \tag{A11c}$$

$$\tilde{M}_\pm^n = \pi^{-3/2}\int_{-\infty}^{\infty} \tilde{\xi}^n g_\pm d\tilde{\xi}, \tag{A12}$$

from the conservation equations.

Let $\tilde{x}^{(i)}$ and $\tilde{\xi}^{(j)}$ be a uniform $\tilde{x}$ grid system and a uniform $\tilde{\xi}$ grid system, respectively. The way of computation for the above formula is as follows: In the first step, the macroscopic variables at the grid $\tilde{x}^{(i)}$ are computed from $\boldsymbol{\Phi}(\tilde{x}^{(i)}, \tilde{\xi}^{(j)}, 0)$ by Simpson's rule, their space derivatives at the grid are computed from the values at $\tilde{x} = \tilde{x}^{(i\pm m)}$ $(m = 1, 2)$ by a finite difference formula, and $\boldsymbol{h}_1(\tilde{x}^{(i)}, \tilde{\xi}^{(j)})$ is computed according to Eqs. (A7a), (A9)–(A11). In the second step, compute the nearest grid from $\tilde{x}_0^{(i,j)}$ $(\equiv \tilde{x}^{(i)} - \Delta\tilde{t}\tilde{\xi}^{(j)})$ and let it be $\tilde{x}^{(P(i,j))}$. Compute $\boldsymbol{h}_1(\tilde{x}_0^{(i,j)}, \tilde{\xi}^{(j)})$ from the values of $\boldsymbol{h}_1(\tilde{x}^{(P(i,j)\pm m)}, \tilde{\xi}^{(j)})$ $(m = 0, 1, 2, 3)$ by using the interpolation formula derived from the Taylor expansion around $\tilde{x}^{(P(i,j))}$. The truncation error of the interpolation formula is $O(\Delta\tilde{x}^7)$, where $\Delta\tilde{x}$ is the width of $\tilde{x}$ grid.

The formula of the splitting method with the modified Euler method in the collision step is obtained if all the space derivatives of macroscopic variables are omitted in the final formula and the formula of the conventional splitting method is obtained if all the differential terms are omitted in Eq. (A7a).

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