First/second-order kinetic flux vector splitting scheme and first-order gas-kinetic scheme explanation and derivation

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1 Introduction

Kinetic Flux Vector Splitting (KFVS) scheme is a well-known scheme, having significant influence in many aspects of fluid mechanics. Gas Kinetic Scheme (GKS) proposed by Kun Xu [1] avoids the intrinsic drawback of the KFVS scheme but maintains good robustness, thus is broadly accepted as the basement of many modern schemes. In this note, we will present the derivation of one-dimensional 1st/2nd-order KFVS and 1st-order GKS and how to implement these algorithms. The extended references include the paper on the detailed construction of KFVS and GKS [2], the connection of the GKS solver with the exact Riemann solver and artificial viscosity [3], and the book on the direct modeling of CFD method (especially for rarefied flow) [4].

2 1st-order KFVS scheme

2.1 Derivation

The KFVS scheme is based on the collisionless Boltzmann equation, its one-dimensional form can be written as

$$f_t + u f_x = 0 \tag{1}$$

from (1) we can use the distribution function at $t = 0$ to replace the original one

$$f(x, t) = f(x - ut, 0) \tag{2}$$

for the one-dimensional Riemann problem, at the moment $t = 0$ we have a dramatic change of conservative variables (denoting by $\mathbf{W}$, as it is a vector consisting of density ρ momentum ρU and energy ρE) in the interface between two cells in the following form

$$\mathbf{W} = \begin{cases} \mathbf{W}^l, & x \leq 0 \\ \mathbf{W}^r, & x > 0 \end{cases} \tag{3}$$

this macroscopic value can be obtained by integrate the Maxwell distribution function on the velocity space

$$\mathbf{W}^l = \int_{-\infty}^{\infty} \left(\int_0^{\infty} \mathbf{\Psi}_\alpha g^l \mathrm{d}u \right) \mathrm{d}\xi$$

$$\mathbf{W}^r = \int_{-\infty}^{\infty} \left(\int_{-\infty}^0 \mathbf{\Psi}_\alpha g^r \mathrm{d}u \right) \mathrm{d}\xi$$

(4)

In which $\mathbf{\Psi}_\alpha = (1, U, 0.5(U^2 + \varepsilon^2))^T$ is the components of the vector of moments. To recover the macroscopic distribution in (4), the microscopic distribution function needs to have a form of

$$f_0 = \begin{cases} g^l, & x \leq 0 \\ g^r, & x \geq 0 \end{cases}$$

(5)

where g represents Maxwell-Boltzmann distribution function. Because the Maxwell distribution has a form of

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

(6)

In which for one-dimensional problem,

$$K = N + 2 = \frac{3 - \gamma}{\gamma - 1}$$

$$\lambda = \frac{K+1}{4} \frac{1}{\rho E / \rho - U^2 / 2}$$

(7)

where K is the degree of freedom, N is the internal degree of freedom, and γ is the specific heat ratio. $N=0$ for monatomic gas, such as He(helium), and $N=2$ for diatomic gas, such as air, O_2(oxygen). And from (1) we know

$$\mathbf{W}_t = -\mathbf{F}_x$$

(8)

Therefore, by introducing the following notation whose explicit form is given in Appendix A

$$< \cdots > = \frac{1}{\rho} \int \int (\cdots) g \mathrm{d}u \mathrm{d}\xi$$

(9)

The final macroscopic variable update formula can thus be obtained by the following expressions

$$\mathbf{W}_j^{n+1} = \mathbf{W}_j^n + \frac{1}{\Delta x} \cdot \int_0^{\Delta t} \left(\mathbf{F}_{j-1/2} - \mathbf{F}_{j+1/2} \right) \mathrm{d}t$$

(10)

$$F = \int_{-\infty}^{\infty} d\xi \int_0^{\infty} u \psi_\alpha g^l du + \int_{-\infty}^{\infty} d\xi \int_{-\infty}^0 u \psi_\alpha g^r du$$

$$= \rho^l \left\langle u^1 \psi_\alpha \right\rangle_{u>0}^l + \rho^r \left\langle u^1 \psi_\alpha \right\rangle_{u<0}^r$$

$$= \rho^l \begin{pmatrix} \left\langle u^1 \right\rangle_{u>0}^l \\ \left\langle u^2 \right\rangle_{u>0}^l \\ \left\langle u^3 \right\rangle_{u>0}^l + \left\langle u^1 \right\rangle_{u>0}^l \left\langle \xi^2 \right\rangle \end{pmatrix}$$

$$+ \rho^r \begin{pmatrix} \left\langle u^1 \right\rangle_{u<0}^r \\ \left\langle u^2 \right\rangle_{u<0}^r \\ \left\langle u^3 \right\rangle_{u<0}^r + \left\langle u^1 \right\rangle_{u<0}^r \left\langle \xi^2 \right\rangle \end{pmatrix}$$

(11)

2.2 Algorithm

From the derivation above, the complete process of 1st-order KFVS scheme can be obtained.

Step 1. Initialization Setting the boundary conditions and initial conditions. In this step, the value of macroscopic variables in every cell will be initialized.

Step 2. Reconstruction For 1st-order schemes, The macroscopic variable keeps the same inside a cell. Therefore, the value of flow variable at the interface is reconstructed as the mean value of the belonging cell, which means at the interface

$$\mathbf{W}^l_{\alpha,j+1/2} = (\mathbf{W}_{\alpha,j+1/2})_- = \overline{\mathbf{W}}_{\alpha,j}$$
$$\mathbf{W}^r_{\alpha,j+1/2} = (\mathbf{W}_{\alpha,j+1/2})_- = \overline{\mathbf{W}}_{\alpha,j+1}$$

Step 3. Flux calculation The flux at every interface is

$$\mathbf{F} = \int_\infty^\infty \mathrm{d}\xi \int_0^\infty u\Psi_\alpha g^l(1 - a^l ut)\mathrm{d}u + \int_{-\infty}^\infty \mathrm{d}\xi \int_{-\infty}^0 u\Psi_\alpha g^r(1 - a^r ut)\mathrm{d}u$$
$$= \rho^l < u^1\Psi_\alpha >^l_{u>0} + \rho^r < u^1\Psi_\alpha >^r_{u<0}$$

The intergral $< u^p >$ and $< \xi^p >$ can be decided by recursion correlations which are given in Appendix A.

Step 4. Variable Update According to the calculation above, the macroscopic variables can be updated by

$$\mathbf{W}^{n+1}_j = \mathbf{W}^n_j + \frac{1}{\Delta x} \cdot \int_0^{\Delta t} \left(\mathbf{F}_{j-1/2} - \mathbf{F}_{j+1/2} \right) \mathrm{d}t \tag{12}$$

3 2nd-order KFVS scheme

3.1 Derivation

To reach higher-order accuracy, on the basement of the 1st-order KFVS scheme the variable reconstruction technique is used to build a 2nd-order KFVS scheme. We construct the flow variable distribution along the both sides of a cell interface

$$\mathbf{W} = \begin{cases} \mathbf{W}^l(1 + \frac{\partial \mathbf{W}^l}{\partial x}x), & x \leq 0 \\ \mathbf{W}^r(1 + \frac{\partial \mathbf{W}^r}{\partial x}x), & x > 0 \end{cases} \tag{13}$$

in such way, every conservative variable has a constant slope inside each cell. To recover the macroscopic distribution in (38), the microscopic distribution function needs to have a form of

$$f_0 = \begin{cases} g^l(1 + a^l x), & x \leq 0 \\ g^r(1 + a^r x), & x \geq 0 \end{cases} \tag{14}$$

3

where $a = g_x/g$. Because the Maxwell distribution has the form of

$$g = \rho \left(\frac{\lambda}{\pi}\right)^{\frac{K+1}{2}} e^{-\lambda\left((u-U)^2+\xi^2\right)} \tag{15}$$

the derivative can thus be obtained by

$$
\begin{aligned}
a = \frac{\partial g/\partial x}{g} &= \frac{\partial(\ln g)}{\partial x} = \frac{\partial}{\partial x}\left(\ln\rho + \frac{K+1}{2}\ln\frac{\lambda}{\pi} - \lambda\left((u-U)^2+\xi^2\right)\right)\\
&= \frac{1}{\rho}\frac{\partial\rho}{\partial x} + \frac{K+1}{2\lambda}\frac{\partial\lambda}{\partial x} - \frac{\partial\lambda}{\partial x}\left((u-U)^2+\xi^2\right) - \lambda\left(2(U-u)\frac{\partial U}{\partial x}\right)\\
&= \frac{1}{\rho}\frac{\partial\rho}{\partial x} - 2\lambda U\frac{\partial U}{\partial x} + \left(\frac{K+1}{2}-U^2\right)\frac{\partial\lambda}{\partial x}\\
&\quad + 2\left(\lambda\frac{\partial U}{\partial x} + U\frac{\partial\lambda}{\partial x}\right)\cdot u - 2\frac{\partial\lambda}{\partial x}\cdot\left(\frac{u^2+\xi^2}{2}\right)\\
&= a_1 + a_2 u + a_3\frac{u^2+\xi^2}{2}
\end{aligned}
\tag{16}
$$

In which

$$
\begin{aligned}
\frac{\partial U}{\partial x} &= \frac{1}{\rho}\left(\frac{\partial(\rho U)}{\partial x} - U\frac{\partial\rho}{\partial x}\right)\\
\frac{\partial\lambda}{\partial x} &= \frac{\partial}{\partial x}\left(\frac{K+1}{4}\left(\frac{1}{\frac{\rho E}{\rho}-U^2/2}\right)\right)\\
&= \frac{K+1}{4}\frac{1}{\left(\frac{\rho E}{\rho}-U^2/2\right)^2}\left(-\frac{1}{\rho}\frac{\partial(\rho E)}{\partial x} + \frac{\rho E}{\rho^2}\frac{\partial\rho}{\partial x} + U\frac{\partial U}{\partial x}\right)
\end{aligned}
\tag{17}
$$

Therefore coefficients a_1, a_2 and a_3 can be obtained by combining derivatives of conservative variables. After acquiring the expression of a, (39) can be transferred to be

$$
\begin{aligned}
\mathbf{W}^l &= \int_{-\infty}^{\infty}\left(\int_0^{\infty}\mathbf{\Psi}_\alpha g^l a^l \mathrm{d}u\right)\mathrm{d}\xi\\
\mathbf{W}^r &= \int_{-\infty}^{\infty}\left(\int_{-\infty}^0\mathbf{\Psi}_\alpha g^r a^r \mathrm{d}u\right)\mathrm{d}\xi
\end{aligned}
\tag{18}
$$

Besides this, there exists other approaches to obtain the coefficient a. For example, introducing the following notation whose form is given in Appendix A

$$<\cdots> = \frac{1}{\rho}\int\int(\cdots)g\mathrm{d}u\mathrm{d}\xi \tag{19}$$

And by applying (41), (43) can be adopted to

$$
\begin{aligned}
\frac{\partial\mathbf{W}}{\partial x} &= \begin{pmatrix}\partial(\rho)/\partial x\\ \partial(\rho U)/\partial x\\ \partial(\rho E)/\partial x\end{pmatrix}\\
&= \begin{pmatrix}
<u^0> & <u^1> & <\frac{u^2+\xi^2}{2}>\\
<u^1> & <u^2> & <\frac{u^3+u^1\xi^2}{2}>\\
<\frac{u^2+\xi^2}{2}> & <\frac{u^3+u^1\xi^2}{2}> & <\frac{u^4+2u^2\xi^2+\xi^4}{4}>
\end{pmatrix}\cdot\begin{pmatrix}a_1\\ a_2\\ a_3\end{pmatrix}
\end{aligned}
\tag{20}
$$

4

In the derivative calculation, slope limiters are frequently used to maintain the stability and accuracy of the calculation. The van Leer limiter is a typical one of them. For a macroscopic variable W, it has the form of

$$\frac{\partial W_j}{\partial x} = L(s, r) = (\text{sign}(s) + \text{sign}(r))\frac{sr}{|s| + |r|} \qquad (21)$$

where s and r can be denoted by

$$\begin{aligned} s &= \frac{W_{j+1} - W_j}{x_{j+1} - x_j} \\ r &= \frac{W_j - W_{j-1}}{x_j - x_{j-1}} \end{aligned} \qquad (22)$$

After attaining the explicit expressions for these coefficients, at the interface, by combining (2) and (38), we have

$$f(x = j + 1/2, t) = f(x - ut, 0)|_{x=0} = \begin{cases} g^l(1 - a^l ut), & u \geq 0 \\ g^r(1 - a^r ut), & u < 0 \end{cases} \qquad (23)$$

And from (1) we know

$$\mathbf{W}_t = -\mathbf{F}_x \qquad (24)$$

Therefore, the final macroscopic variable update formula can thus be obtained by the following expressions

$$\mathbf{W}_j^{n+1} = \mathbf{W}_j^n + \frac{1}{\Delta x} \cdot \int_0^{\Delta t} \left(\mathbf{F}_{j-1/2} - \mathbf{F}_{j+1/2}\right) \mathrm{d}t \qquad (25)$$

$$\begin{aligned} \mathbf{F} &= \int_{-\infty}^{\infty} \mathrm{d}\xi \int_0^{\infty} u\mathbf{\Psi}_\alpha g^l(1 - a^l ut)\mathrm{d}u + \int_{-\infty}^{\infty} \mathrm{d}\xi \int_{-\infty}^0 u\mathbf{\Psi}_\alpha g^r(1 - a^r ut)\mathrm{d}u \\ &= \rho^l < u^1\mathbf{\Psi}_\alpha >_{u>0}^l + \rho^r < u^1\mathbf{\Psi}_\alpha >_{u<0}^r \\ &\quad - \rho^l t < u^2 a^l\mathbf{\Psi}_\alpha >_{u>0}^l - \rho^r t < u^2 a^r\mathbf{\Psi}_\alpha >_{u<0}^r \end{aligned} \qquad (26)$$

3.2 Algorithm

From the derivation above, the complete process of 2nd-order KFVS scheme can be obtained.

Step 1. Initialization Setting the boundary conditions and initial conditions. In this step, the value of macroscopic variables in every cell will be initialized.

Step 2. Reconstruction Decide the derivatives of macroscopic variable $\{\partial\rho/\partial x, \partial\rho U/\partial x, \partial\rho E/\partial x\}^T$. Limiters might be used in this step, like the van Leer limiter

$$\frac{\partial W_j}{\partial x} = L(s, r) = (\text{sign}(s) + \text{sign}(r))\frac{sr}{|s| + |r|}$$

where s and r can be denoted by

$$s = \frac{W_{j+1} - W_j}{x_{j+1} - x_j}$$

$$r = \frac{W_j - W_{j-1}}{x_j - x_{j-1}}$$

After obtaining the derivatives, the macroscopic value of every cell can be reconstructed, and the value at the interface is

$$\mathbf{W}^l_{\alpha,j+1/2} = (\mathbf{W}_{\alpha,j+1/2})_- = \overline{\mathbf{W}}_{\alpha,j} + \frac{\partial \mathbf{W}_{\alpha,j}}{\partial x}\frac{\Delta x}{2}$$

$$\mathbf{W}^l_{\alpha,j+1/2} = (\mathbf{W}_{\alpha,j+1/2})_+ = \overline{\mathbf{W}}_{\alpha,j+1} - \frac{\partial \mathbf{W}_{\alpha,j+1}}{\partial x}\frac{\Delta x}{2}$$

Step 3. Coefficients calculation   The slope of macroscopic variables can be decided by (41). The exact form is

$$a^l = a^l_1 + a^l_2 \cdot u + a^l_3 \cdot \frac{u^2 + \xi^2}{2}$$

$$a^r = a^r_1 + a^r_2 \cdot u + a^r_3 \cdot \frac{u^2 + \xi^2}{2}$$

$$a_1 = \frac{1}{\rho}\frac{\partial \rho}{\partial x} - 2\lambda U \frac{\partial U}{\partial x} + \left(\frac{K+1}{2} - U^2\right)\frac{\partial \lambda}{\partial x}$$

$$a_2 = 2\left(\lambda\frac{\partial U}{\partial x} + U\frac{\partial \lambda}{\partial x}\right)$$

$$a_3 = -2\frac{\partial \lambda}{\partial x}$$

In which

$$\frac{\partial U}{\partial x} = \frac{1}{\rho}\left(\frac{\partial(\rho U)}{\partial x} - U\frac{\partial \rho}{\partial x}\right)$$

$$\frac{\partial \lambda}{\partial x} = \frac{\partial}{\partial x}\left(\frac{K+1}{4}\left(\frac{1}{\frac{\rho E}{\rho} - U^2/2}\right)\right) \qquad (27)$$

$$= \frac{K+1}{4}\frac{1}{\left(\frac{\rho E}{\rho} - U^2/2\right)^2}\left(-\frac{1}{\rho}\frac{\partial(\rho E)}{\partial x} + \frac{\rho E}{\rho^2}\frac{\partial \rho}{\partial x} + U\frac{\partial U}{\partial x}\right)$$

Step 4. Flux calculation   The flux at every interface is

$$\mathbf{F} = \int_\infty^\infty \mathrm{d}\xi \int_0^\infty u\Psi_\alpha g^l(1 - a^l ut)\mathrm{d}u + \int_{-\infty}^\infty \mathrm{d}\xi \int_{-\infty}^0 u\Psi_\alpha g^r(1 - a^r ut)\mathrm{d}u$$

$$= \rho^l < u^1\Psi_\alpha >^l_{u>0} + \rho^r < u^1\Psi_\alpha >^r_{u<0}$$

$$- \rho^l t < u^2 a^l \Psi_\alpha >^l_{u>0} - \rho^r t < u^2 a^r \Psi_\alpha >^r_{u<0}$$

note that the ρ here has been reconstructed. The intergral$< u^p >$and$< \xi^p >$ can be decided by the recursion correlations presented in Appendix A.

Step 5. Variable Update According to the calculation above, the macroscopic variables can be updated by

$$\mathbf{W}_j^{n+1} = \mathbf{W}_j^n + \frac{1}{\Delta x} \cdot \int_0^{\Delta t} \left(\mathbf{F}_{j-1/2} - \mathbf{F}_{j+1/2}\right) \mathrm{d}t \tag{28}$$

4   1st-order Gas Kinetic Scheme

4.1   Derivation

Using the Bhatnagar-Gross-Krook (BGK) model, the Boltzmann equation with collision term becomes

$$f_t + u f_x = -\frac{f - g}{\tau} \tag{29}$$

The zeroth-order integral form of it is

$$f(x,t) = \left(1 - e^{-\frac{t-t_0}{\tau}}\right) g^c + e^{-\frac{t-t_0}{\tau}} g^{l,r} \tag{30}$$

where

$$\begin{aligned}
&\int_{-\infty}^{\infty} \mathrm{d}\xi \int_{-\infty}^{\infty} \mathbf{\Psi}_\alpha g^c \mathrm{d}u \\
&= \int_{-\infty}^{\infty} \mathrm{d}\xi \int_0^{\infty} \mathbf{\Psi}_\alpha g^l \mathrm{d}u + \int_{-\infty}^{\infty} \mathrm{d}\xi \int_{-\infty}^0 \mathbf{\Psi}_\alpha g^r \mathrm{d}u
\end{aligned} \tag{31}$$

In this way, the total flux will be divided into two parts, the first one is the same with 1st-order KFVS

$$\begin{aligned}
\mathbf{F}_{0,j+1/2} &= \int_{-\infty}^{\infty} \mathrm{d}\xi \int_0^{\infty} \mathbf{\Psi}_\alpha g^l u \mathrm{d}u + \int_{-\infty}^{\infty} \mathrm{d}\xi \int_{-\infty}^0 \mathbf{\Psi}_\alpha g^r u \mathrm{d}u \\
&= \rho^l \cdot \begin{pmatrix} < u^1 >_{u>0}^l \\ < u^2 >_{u>0}^l \\ < \frac{1}{2}(u^3 + u^1 \xi^2) >_{u>0}^l \end{pmatrix} \\
&+ \rho^r \cdot \begin{pmatrix} < u^1 >_{u<0}^r \\ < u^2 >_{u<0}^r \\ < \frac{1}{2}(u^3 + u^1 \xi^2) >_{u<0}^r \end{pmatrix}
\end{aligned} \tag{32}$$

To obtain the second part of flux, we need to get the macroscopic variables at the interfaces first

$$\begin{aligned}
\begin{pmatrix} \rho^c \\ \rho^c U^c \\ \rho^c E^c \end{pmatrix} &= \rho^l \cdot \begin{pmatrix} < u^0 >_{u>0}^l \\ < u^1 >_{u>0}^l \\ < \frac{1}{2}(u^2 + u^0 \xi^2) >_{u>0}^l \end{pmatrix} + \rho^r \cdot \begin{pmatrix} < u^0 >_{u<0}^r \\ < u^1 >_{u<0}^r \\ < \frac{1}{2}(u^2 + u^0 \xi^2) >_{u<0}^r \end{pmatrix} \\
&= \rho^l \begin{pmatrix} \langle u^0 \rangle_{u>0}^l \\ \langle u^1 \rangle_{u>0}^l \\ \frac{1}{2}(\langle u^2 \rangle_{u>0}^l + \langle u^0 \rangle_{u>0}^l \langle \xi^2 \rangle) \end{pmatrix} + \rho^r \begin{pmatrix} \langle u^0 \rangle_{u<0}^r \\ \langle u^1 \rangle_{u<0}^r \\ \frac{1}{2}(\langle u^2 \rangle_{u<0}^r + \langle u^0 \rangle_{u<0}^r \langle \xi^2 \rangle) \end{pmatrix}
\end{aligned} \tag{33}$$

then from (33) we can obtain

$$
\begin{aligned}
U^c &= \frac{\rho^c U^c}{\rho^c} \\
\lambda^c &= \frac{K+1}{4} \frac{\rho^c}{\rho^c E^c - \frac{1}{2\rho^c}\left(\rho^c U^c\right)^2}
\end{aligned}
\tag{34}
$$

Then we can calculate the second part of flux according to the interface macroscopic variables, U^c and λ^c obtained from (33) and (34)

$$
\begin{aligned}
\mathbf{F}_{1,j+1/2} &= \int_{-\infty}^{\infty} \mathrm{d}\xi \int_{-\infty}^{\infty} \boldsymbol{\Psi}_\alpha g_0 u \mathrm{d}u \\
&= \rho^c \cdot \begin{pmatrix} <u^1>^c \\ <u^2>^c \\ <\frac{1}{2}(u^3 + u^1\xi^2)>^c \end{pmatrix}
\end{aligned}
\tag{35}
$$

then with the notation $\eta = e^{-t/\tau}$, we can finally get the 1st order GKS flux

$$
\mathbf{F}_{j+1/2} = (1-\eta)\mathbf{F}_{1,j+1/2} + \eta\mathbf{F}_{0,j+1/2}
\tag{36}
$$

then macroscopic variables can be updated by

$$
\mathbf{W}_j^{n+1} - \mathbf{W}_j^n = \frac{1}{\Delta x} \cdot \int_0^{\Delta t} \left(\mathbf{F}_{j-1/2} - \mathbf{F}_{j+1/2}\right) \mathrm{d}t
\tag{37}
$$

Through derivation we can obtain the explicit form of $F_{j-1/2}$ and $F_{j+1/2}$. Due to its enormous length, the exact form will be provided as attachment.

4.2 Algorithm

From the derivation above, the complete process of 1st-order GKS scheme can be obtained.

Step 1. Initialization Setting the boundary conditions and initial conditions. In this step, the value of macroscopic variables in every cell will be initialized.

Step 2. Reconstruction For 1st-order schemes, The macroscopic variable keeps the same inside a cell. Therefore, the value of flow variable at the interface is reconstructed as the mean value of the belonging cell, which means at the interface

$$
\begin{aligned}
\mathbf{W}_{\alpha,j+1/2}^l &= (\mathbf{W}_{\alpha,j+1/2})_- = \overline{\mathbf{W}}_{\alpha,j} \\
\mathbf{W}_{\alpha,j+1/2}^r &= (\mathbf{W}_{\alpha,j+1/2})_+ = \overline{\mathbf{W}}_{\alpha,j+1}
\end{aligned}
$$

Step 3. Equilibrium state calculation From the initial macroscopic variable distribution, after reconstruction, the equilibrium state in (33) becomes

$$
\begin{pmatrix} \rho^c_{j+1/2} \\ \rho^c_{j+1/2} U^c_{j+1/2} \\ \rho^c_{j+1/2} E^c_{j+1/2} \end{pmatrix} = \rho^l_{j+1/2} \cdot \begin{pmatrix} < u^0 >^l_{u>0} \\ < u^1 >^l_{u>0} \\ < \frac{1}{2}(u^2 + \xi^2) >^l_{u>0} \end{pmatrix}
$$

$$
+ \rho^r_{j+1/2} \cdot \begin{pmatrix} < u^0 >^r_{u<0} \\ < u^1 >^r_{u<0} \\ < \frac{1}{2}(u^2 + \xi^2) >^r_{u<0} \end{pmatrix}
$$

thus the primary variables in (34) become

$$
U^c_{j+1/2} = \frac{\rho^c_{j+1/2} U^c_{j+1/2}}{\rho^c_{j+1/2}}
$$

$$
\lambda^c_{j+1/2} = \frac{K+1}{4} \frac{\rho^c_{j+1/2}}{\rho^c_{j+1/2} E^c_{j+1/2} - \frac{1}{2\rho^c_{j+1/2}} (\rho^c_{j+1/2} U^c_{j+1/2})^2}
$$

Step 4. Flux calculation With the notation $\eta = e^{-t/\tau}$, the flux at every interface is consisted of two parts

$$
\mathbf{F}_{j+1/2} = (1 - \eta) \mathbf{F}_{1,j+1/2} + \eta \mathbf{F}_{0,j+1/2}
$$

the form of the first part is the same as 1st-order KFVS scheme

$$
\mathbf{F}_{0,j+1/2} = \int d\xi \int_{u>0} \boldsymbol{\Psi}_\alpha g^l u du + \int d\xi \int_{u<0} \boldsymbol{\Psi}_\alpha g^r u du
$$

$$
= \rho^l_{j+1/2} \cdot \begin{pmatrix} < u^1 >^l_{u>0} \\ < u^2 >^l_{u>0} \\ < \frac{1}{2}(u^3 + u^1 \xi^2) >^l_{u>0} \end{pmatrix}
$$

$$
+ \rho^r_{j+1/2} \cdot \begin{pmatrix} < u^1 >^r_{u<0} \\ < u^2 >^r_{u<0} \\ < \frac{1}{2}(u^3 + u^1 \xi^2) >^r_{u<0} \end{pmatrix}
$$

where the intergral$< u^p >$and$< \xi^p >$ can be decided by recursion correlations. The second part needs to be calculated from equilibrium state variables

$$
\mathbf{F}_{1,j+1/2} = \int d\xi \int \boldsymbol{\Psi}_\alpha g_0 u du
$$

$$
= \rho^c_{j+1/2} \cdot \begin{pmatrix} < u^1 >^c \\ < u^2 >^c \\ < \frac{1}{2}(u^3 + u^1 \xi^2) >^c \end{pmatrix}
$$

Step 5. Variable update According to the calculation above, the macroscopic variables can be updated by

$$
\begin{aligned}
\mathbf{W}_j^{n+1} - \mathbf{W}_j^n ={}& \frac{1}{\Delta x} \cdot \int_0^{\Delta t} \left(\mathbf{F}_{j-1/2} - \mathbf{F}_{j+1/2} \right) \mathrm{d}t \\
={}& \frac{1}{\Delta x} \cdot \int_0^{\Delta t} \left[(1-\eta)\mathbf{F}_{1,j-1/2} + \eta\mathbf{F}_{0,j-1/2} \right] \mathrm{d}t \\
& - \frac{1}{\Delta x} \cdot \int_0^{\Delta t} \left[(1-\eta)\mathbf{F}_{1,j+1/2} + \eta\mathbf{F}_{0,j+1/2} \right] \mathrm{d}t \\
={}& \frac{1}{\Delta x} \cdot \left[(\Delta t - \tau(1-\eta))\mathbf{F}_{1,j-1/2} + (\tau(1-\eta)\mathbf{F}_{0,j-1/2}) \right] \\
& - \frac{1}{\Delta x} \cdot \left[(\Delta t - \tau(1-\eta))\mathbf{F}_{1,j+1/2} + (\tau(1-\eta)\mathbf{F}_{0,j+1/2}) \right]
\end{aligned}
$$

In practice, the collision time τ is modified to the numerical collision time τ_n to simulate the invicid flow with discontinuity. Usually $\eta = \tau_n/p$ can be chosen as a constant, e.g., 0.3, and the 1st-order GKS will be essentially positive-preserving as proven in [5].

5 2nd-order GKS Kinetic scheme

5.1 Derivation

For the BGK model, the equivalent integral solution of f at the cell interface and time t is

$$
\begin{aligned}
f(x,t,u,\xi) ={}& (1 - e^{-t/\tau_n})g^c + ((t+\tau)e^{-t/\tau_n} - \tau)a^c u g^c + (t - \tau + \tau e^{-t/\tau_n})A^c g^c \\
& + e^{-t/\tau_n} g^{l/r} \left[1 - (t+\tau)a^{l/r}u_i - \tau A^{l/r} \right],
\end{aligned}
\tag{38}
$$

where

$$
\int_{-\infty}^{\infty} d\xi \int_{-\infty}^{\infty} \psi_\alpha g^c du = \int_{-\infty}^{\infty} d\xi \int_0^{\infty} \psi_\alpha g^l du + \int_{-\infty}^{\infty} d\xi \int_{-\infty}^0 \psi_\alpha g^r du.
\tag{39}
$$

Due to the limitation of mesh size, the collision time cannot provide enough numerical dissipation to enlarge the shock thickness to the mesh size scale. τ is enlarged as

$$
\tau_n = \tau + c_2 \left| \frac{p_l - p_r}{p_l + p_r} \right| \Delta t = \frac{\mu}{p} + c_2 \left| \frac{p_l - p_r}{p_l + p_r} \right| \Delta t.
\tag{40}
$$

For the inviscid flow,

$$
\tau_n = c_1 \Delta t + c_2 \left| \frac{p_l - p_r}{p_l + p_r} \right| \Delta t,
\tag{41}
$$

where $c_1 = 0.05$ and $c_2 = 1$ usually. And $a^c = g_x^c/g^c (a^{l/r} = g_x^{l/r}/g^{l/r}, A^c = g_t^c/g^c, A^{l/r} = g_t^{l/r}/g^{l/r})$, which can be gotten by the equation (16).According to the spatial derivatives of macroscopic flow variables and the compatibility condition, there is

$$
\begin{aligned}
\langle a^c \rangle &= \frac{\partial W}{\partial x}, \\
\langle A^c + a^c u \rangle &= 0.
\end{aligned}
\tag{42}
$$

The total flux can be divided into two parts, $F_{0j+1/2}$ and $F_{1j+1/2}$, just like the way in section 4.1,

$$
\begin{aligned}
F_{0,j+1/2} &= \int_{-\infty}^{\infty} d\xi \int_{0}^{\infty} \psi_\alpha g^l u \left[1 - (t+\tau)a^l u - \tau A^l \right] du \\
&\quad + \int_{-\infty}^{\infty} d\xi \int_{-\infty}^{0} \psi_\alpha g^r u \left[1 - (t+\tau)a^r u - \tau A^r \right] du \\
&= \rho^l \left[\langle u^1 \psi_\alpha \rangle_{u>0}^{l} - \langle (t+\tau)a^l u^2 \psi_\alpha \rangle_{u>0}^{l} - \langle \tau A^l u^1 \psi_\alpha \rangle_{u>0}^{l} \right] \\
&\quad + \rho^r \left[\langle u^1 \psi_\alpha \rangle_{u<0}^{r} - \langle (t+\tau)a^r u^2 \psi_\alpha \rangle_{u<0}^{r} - \langle \tau A^r u^1 \psi_\alpha \rangle_{u<0}^{r} \right].
\end{aligned}
\tag{43}
$$

To obtain the second part of flux, we need to get the macroscopic variables at the interface first, based on the equation (33) and (34). The second part of the flux is

$$
\begin{aligned}
F_{1,j+1/2} &= \int_{-\infty}^{\infty} d\xi \int_{0}^{\infty} \psi_\alpha g^c u \left[\begin{array}{c} (1 - e^{-t/\tau_n}) + ((t+\tau)e^{-t/\tau_n} - \tau)a^c u \\ + (t - \tau + \tau e^{-t/\tau_n})A^c \end{array} \right] du \\
&= \rho^c \left[\begin{array}{c} \langle (1 - e^{-t/\tau_n})u^1 \psi_\alpha \rangle^{c} - \langle ((t+\tau)e^{-t/\tau_n} - \tau)a^c u^2 \psi_\alpha \rangle^{c} \\ - \langle (t - \tau + \tau e^{-t/\tau_n})A^c u^1 \psi_\alpha \rangle^{c} \end{array} \right].
\end{aligned}
\tag{44}
$$

Then with the notation $\eta = e^{-t/\tau_n}$, the total flux can be obtained,

$$
F_{j+1/2} = F_{1,j+1/2} + \eta \cdot F_{0,j+1/2}
\tag{45}
$$

and the macroscopic variables can be updated by

$$
W_j^{n+1} = W_j^n + \frac{1}{\Delta x} \cdot \int_0^{\Delta t} (F_{j-1/2} - F_{j+1/2}) dt
\tag{46}
$$

5.2 Algorithm

From the derivation above, the complete process of 2nd-order GKS scheme can be obtained.

Step 1. Initialization Setting the boundary conditions and initial conditions. In this step, the value of macroscopic variables in every cell will be initialized.

Step 2. Reconstruction Decide the derivatives of macroscopic variable $\{\partial \rho / \partial x, \partial \rho U / \partial x, \partial \rho E / \partial x\}^T$. Limiters might be used in this step, like the van Leer limiter. After obtaining the derivatives, the macroscopic value of every cell can be reconstructed, and the value at the interface is

$$
\begin{aligned}
\mathbf{W}_{\alpha,j+1/2}^{l} &= (\mathbf{W}_{\alpha,j+1/2})_{-} = \overline{\mathbf{W}}_{\alpha,j} + \frac{\partial \mathbf{W}_{\alpha,j}}{\partial x} \frac{\Delta x}{2} \\
\mathbf{W}_{\alpha,j+1/2}^{l} &= (\mathbf{W}_{\alpha,j+1/2})_{+} = \overline{\mathbf{W}}_{\alpha,j+1} - \frac{\partial \mathbf{W}_{\alpha,j+1}}{\partial x} \frac{\Delta x}{2}
\end{aligned}
$$

Step 3. Equilibrium state calculation Refer to the step 3 in section 4.2 here.

Step 4. Coefficients calculation The coefficients needed in calculation can be decided by(16),

$$a^{l/r} = a_1^{l/r} + a_2^{l/r} \cdot u + a_3^{l/r} \cdot \frac{u^2 + \xi^2}{2}$$

$$A^{l/r} = A_1^{l/r} + A_2^{l/r} \cdot u + A_3^{l/r} \cdot \frac{u^2 + \xi^2}{2}$$

$$a^c = a_1^c + a_2^c \cdot u + a_3^c \cdot \frac{u^2 + \xi^2}{2}$$

$$A^c = A_1^c + A_2^c \cdot u + A_3^c \cdot \frac{u^2 + \xi^2}{2}$$

$$a_1 = \frac{1}{\rho}\frac{\partial \rho}{\partial x} - 2\lambda U \frac{\partial U}{\partial x} + (\frac{K+1}{2} - U^2)\frac{\partial \lambda}{\partial x}, a_2 = 2(\lambda \frac{\partial U}{\partial x} + U \frac{\partial \lambda}{\partial x}), a_3 = -2\frac{\partial \lambda}{\partial x}$$

$$A_1 = \frac{1}{\rho}\frac{\partial \rho}{\partial t} - 2\lambda U \frac{\partial U}{\partial t} + (\frac{K+1}{2} - U^2)\frac{\partial \lambda}{\partial t}, A_2 = 2(\lambda \frac{\partial U}{\partial t} + U \frac{\partial \lambda}{\partial t}), A_3 = -2\frac{\partial \lambda}{\partial t}$$

Besides,

$$\frac{\partial W_{j+1/2}^c}{\partial x} = \rho_{j+1/2}^l \left\langle a^l \psi_\alpha \right\rangle_{u>0}^l + \rho_{j+1/2}^r \left\langle a^r \psi_\alpha \right\rangle_{u<0}^r$$

$$\frac{\partial W_{j+1/2}^{l/r}}{\partial t} = -\rho_{j+1/2}^{l/r} \left\langle a^{l/r} u \psi_\alpha \right\rangle_{u>0/u<0}^{l/r}$$

$$\frac{\partial W_{j+1/2}^c}{\partial t} = -\rho_{j+1/2}^c \left\langle a^c u \psi_\alpha \right\rangle^c$$

Step 5. Flux calculation The flux at every interface is

$$
\begin{aligned}
F_{j+1/2} =& F_{1,j+1/2} + \eta \cdot F_{0,j+1/2} \\
=& \rho^c \left[\begin{array}{l} \left\langle (1 - e^{-t/\tau_n})u^1\psi_\alpha \right\rangle^c - \left\langle ((t+\tau)e^{-t/\tau_n} - \tau)a^c u^2 \psi_\alpha \right\rangle^c \\ - \left\langle (t - \tau + \tau e^{-t/\tau_n})A^c u^1 \psi_\alpha \right\rangle^c \end{array} \right] \\
& + \eta \cdot \rho^l \left[\left\langle u^1\psi_\alpha \right\rangle_{u>0}^l - \left\langle (t+\tau)a^l u^2 \psi_\alpha \right\rangle_{u>0}^l - \left\langle \tau A^l u^1 \psi_\alpha \right\rangle_{u>0}^l \right] \\
& + \eta \cdot \rho^r \left[\left\langle u^1\psi_\alpha \right\rangle_{u<0}^r - \left\langle (t+\tau)a^r u^2 \psi_\alpha \right\rangle_{u<0}^r - \left\langle \tau A^r u^1 \psi_\alpha \right\rangle_{u<0}^r \right] \\
=& (1 - e^{-t/\tau_n})\rho^c \left\langle u^1\psi_\alpha \right\rangle^c \\
& - ((t+\tau)e^{-t/\tau_n} - \tau)\rho^c \left\langle a^c u^2 \psi_\alpha \right\rangle^c \\
& - (t - \tau + \tau e^{-t/\tau_n})\rho^c \left\langle A^c u^1 \psi_\alpha \right\rangle^c \\
& + e^{-t/\tau_n} \left(\rho^l \cdot \left\langle u^1\psi_\alpha \right\rangle_{u>0}^l + \rho^r \cdot \left\langle u^1\psi_\alpha \right\rangle_{u<0}^r \right) \\
& - e^{-t/\tau_n}(t+\tau) \left(\rho^l \cdot \left\langle a^l u^2 \psi_\alpha \right\rangle_{u>0}^l + \rho^r \cdot \left\langle a^r u^2 \psi_\alpha \right\rangle_{u<0}^r \right) \\
& - e^{-t/\tau_n}\tau \left(\rho^l \cdot \left\langle A^l u^1 \psi_\alpha \right\rangle_{u>0}^l + \rho^r \cdot \left\langle A^r u^1 \psi_\alpha \right\rangle_{u<0}^r \right).
\end{aligned}
$$

Step 6. Variable Update According to the calculation above, the macroscopic variables can be updated by

$$
\begin{aligned}
W_j^{n+1} - W_j^n =& \frac{1}{\Delta x} \cdot \int_0^{\Delta t} (F_{j-1/2} - F_{j+1/2}) dt \\
=& \frac{1}{\Delta x} \cdot \int_0^{\Delta t} (F_{1,j-1/2} + \eta \cdot F_{0,j-1/2}) dt \\
& - \frac{1}{\Delta x} \cdot \int_0^{\Delta t} (F_{1,j+1/2} + \eta \cdot F_{0,j+1/2}) dt.
\end{aligned}
\tag{47}
$$

Take the first item at the right side of the equation as an example,

$$
\begin{aligned}
& \int_0^{\Delta t} (F_{1,j-1/2} + \eta \cdot F_{0,j-1/2}) dt \\
=& \int_0^{\Delta t} (1 - e^{-t/\tau_n}) \rho^c \left\langle u^1 \psi_\alpha \right\rangle^c dt \\
& - \int_0^{\Delta t} ((t+\tau) e^{-t/\tau_n} - \tau) \rho^c \left\langle a^c u^2 \psi_\alpha \right\rangle^c dt \\
& - \int_0^{\Delta t} (t - \tau + \tau e^{-t/\tau_n}) \rho^c \left\langle A^c u^1 \psi_\alpha \right\rangle^c dt \\
& + \int_0^{\Delta t} e^{-t/\tau_n} \left(\rho^l \cdot \left\langle u^1 \psi_\alpha \right\rangle_{u>0}^l + \rho^r \cdot \left\langle u^1 \psi_\alpha \right\rangle_{u<0}^r \right) dt \\
& - \int_0^{\Delta t} e^{-t/\tau_n}(t+\tau) \left(\rho^l \cdot \left\langle a^l u^2 \psi_\alpha \right\rangle_{u>0}^l + \rho^r \cdot \left\langle a^r u^2 \psi_\alpha \right\rangle_{u<0}^r \right) dt \\
& - \int_0^{\Delta t} e^{-t/\tau_n} \tau \left(\rho^l \cdot \left\langle A^l u^1 \psi_\alpha \right\rangle_{u>0}^l + \rho^r \cdot \left\langle A^r u^1 \psi_\alpha \right\rangle_{u<0}^r \right) dt \\
=& (\Delta t + \tau_n \eta - \tau_n) \rho^c \left\langle u^1 \psi_\alpha \right\rangle^c \\
& + \left(\tau_n^2 (1-\eta) + \tau_n \tau (1-\eta) - \tau_n \eta \cdot \Delta t - \tau \cdot \Delta t \right) \rho^c \left\langle a^c u^2 \psi_\alpha \right\rangle^c \\
& + \left(\frac{(\Delta t)^2}{2} + \tau_n \tau (1-\eta) - \tau \cdot \Delta t \right) \rho^c \left\langle A^c u^1 \psi_\alpha \right\rangle^c \\
& + \tau_n (1-\eta) \left(\rho^l \cdot \left\langle u^1 \psi_\alpha \right\rangle_{u>0}^l + \rho^r \cdot \left\langle u^1 \psi_\alpha \right\rangle_{u<0}^r \right) \\
& + \left(\tau_n \tau (\eta-1) + \tau_n^2 (\eta-1) + \tau_n \eta \cdot \Delta t \right) \left(\rho^l \cdot \left\langle a^l u^2 \psi_\alpha \right\rangle_{u>0}^l + \rho^r \cdot \left\langle a^r u^2 \psi_\alpha \right\rangle_{u<0}^r \right) \\
& + \tau_n \tau (\eta-1) \left(\rho^l \cdot \left\langle A^l u^1 \psi_\alpha \right\rangle_{u>0}^l + \rho^r \cdot \left\langle A^r u^1 \psi_\alpha \right\rangle_{u<0}^r \right),
\end{aligned}
\tag{48}
$$

and the second item obeys the same rule. In this way, all conservative valuables can be updated.

Appendix A: Recursive Correlations for the Moments Calculation

To deal with the integral of Maxwellian distribution function, we use a unified form of it

$$< \cdots > = \frac{1}{\rho} \int \mathrm{d}\xi \int_{-\infty}^{+\infty} (\cdots) g \mathrm{d}u$$

$$< \cdots >_{u>0} = \frac{1}{\rho} \int \mathrm{d}\xi \int_{0}^{+\infty} (\cdots) g \mathrm{d}u$$

$$< \cdots >_{u<0} = \frac{1}{\rho} \int \mathrm{d}\xi \int_{-\infty}^{0} (\cdots) g \mathrm{d}u$$

During the calculation, we have

$$< u^n \xi^l > = < u^n > < \xi^l >$$

where n is an integer starting from 0 and l is an even integer starting from 0 due to the symmetrical property of Xi. For the moments of $< \xi^l >$, the limits will always be $-\infty$ and $+\infty$, so

$$< \xi^2 > = \frac{K}{2\lambda}$$

$$< \xi^4 > = \frac{K^2 + 2K}{4\lambda^2}$$

For u, the full scope integral has the form

$$< u^0 > = 1$$

$$< u^1 > = U$$

$$\cdots$$

$$< u^{n+2} > = U < u^{n+1} > + \frac{n+1}{2\lambda} < u^n >$$

and the half scope integral has the form

$$< u^0 >_{>0} = \frac{1}{2} \mathrm{erfc} \left(-\sqrt{\lambda} U \right)$$

$$< u^1 >_{>0} = U < u^0 >_{>0} + \frac{1}{2} \frac{e^{-\lambda U^2}}{\sqrt{\pi\lambda}}$$

$$\cdots$$

$$< u^{n+2} >_{>0} = U < u^{n+1} >_{>0} + \frac{n+1}{2\lambda} < u^n >_{>0}$$

and

$$< u^0 >_{<0} = \frac{1}{2} \mathrm{erfc} \left(\sqrt{\lambda} U \right)$$

$$< u^1 >_{<0} = U < u^0 >_{<0} - \frac{1}{2} \frac{e^{-\lambda U^2}}{\sqrt{\pi\lambda}}$$

$$\cdots$$

$$< u^{n+2} >_{<0} = U < u^{n+1} >_{<0} + \frac{n+1}{2\lambda} < u^n >_{<0}$$

where erfc is the error function which can be written as

$$\text{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-\eta^2} \, \mathrm{d}\eta$$

by the recursive correlation above, the moments of Maxwellian distribution function can thus be obtained.

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