Entropy Analysis of Kinetic Flux Vector Splitting Schemes for the Compressible Euler Equations

Shiu Hong Lui * Kun Xu †

Abstract

Flux Vector Splitting (FVS) scheme is one group of approximate Riemann solvers for the compressible Euler equations. In this paper, the discretized entropy condition of the Kinetic Flux Vector Splitting (KFVS) scheme based on the gas-kinetic theory is proved. The proof of the entropy condition involves the entropy definition difference between the distinguishable and indistinguishable particles.

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1 Introduction

There are many numerical approaches to the solution of the Euler equations. Godunov and Boltzmann schemes are two of them [4]. Broadly speaking, Godunov scheme is based on the Riemann solution in the gas evolution stage, and the Boltzmann scheme uses the microscopic particle distribution function as the basis to construct the fluxes. While the construction methodology is different between the Godunov and kinetic schemes, both first order schemes can be written in the framework of the $3-$point conservative methods.

There are mainly two kinds of gas-kinetic schemes, and the differences are in the governing equations in the gas evolution stage. One of the well-known kinetic schemes is called KFVS which is based on the collisionless Boltzmann equation [9, 10], and the other is based on the collisional BGK model [15]. By combining the dynamical effects from the gas evolution stage and projection stage, the real governing equation for both KFVS and BGK schemes are physically the same except the particle collision time τ in the BGK scheme is replaced by the CFL time step Δt in the KFVS scheme [14].

The previous paper [11] analyzed the positivity property, such as positive density and pressure, for the gas-kinetic scheme. In this sequel, we analyze the entropy condition for the first order KFVS schemes.

*Department of Mathematics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong. Email: shlui@uxmail.ust.hk

†Department of Mathematics, Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong. Email: makxu@uxmail.ust.hk

2 Preliminaries

We consider the one dimensional Euler equations of gas dynamics:

$$\begin{cases} \rho_t + m_x = 0, \\ m_t + (mU + p)_x = 0, \\ E_t + (EU + pU)_x = 0, \end{cases} \tag{2.1}$$

where ρ is the density, U the velocity, $m = \rho U$ the momentum, $E = \frac{1}{2}\rho U^2 + \rho e$ the energy per unit mass, e the internal energy density, p the pressure. We assume that the gas is a γ-law gas, i.e., $p = (\gamma - 1)\rho e$. In order to obtain the approximate solution for the above equations, the gas-kinetic scheme solves the Boltzmann equation in the gas evolution stage.

The Boltzmann equation in the 1-D case is [6]

$$f_t + uf_x = Q(f, f),$$

where f is the gas-distribution function, u the particle velocity, and $Q(f, f)$ the collision term. The collision term is an integral function which accounts for the binary collisions. In most cases, the collision term can be simplified and the BGK model is the most successful one [1],

$$Q(f, f) = (g - f)/\tau,$$

where g is the equilibrium state and τ the collision time. For the Euler equations, the equilibrium state g is a Maxwellian,

$$g = \rho \left(\frac{\lambda}{\pi}\right)^{\frac{K+1}{2}} e^{-\lambda((u-U)^2+\xi^2)}, \tag{2.2}$$

where ξ is a K dimensional vector which accounts for the internal degrees of freedom, such as molecular rotation and vibrations, and $\xi^2 = \xi_1^2 + \xi_2^2 + ... + \xi_K^2$. Note that K is related to the specific heat ratio γ,

$$K = (3 - \gamma)/(\gamma - 1).$$

Monotonic gas has $\gamma = 5/3$, and diatomic gas has $\gamma = 1.4$. The lower limit of γ is 1, which corresponds to an infinite number of internal degrees of freedom. For example, $\gamma = 103/101$ is equivalent to $K = 100$, which gives 98 internal degrees of freedom for the molecule. In the equilibrium state, λ is related to the gas temperature T

$$\lambda = \frac{m}{2kT},$$

where m is molecular mass and k the Boltzmann constant.

The connection between the distribution function f and macroscopic flow variables is

$$(\rho, m, E)^T = \int \psi_\alpha f du d\xi,$$

where $d\xi = d\xi_1 d\xi_2 ... d\xi_K$ and

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

are the moments of density ρ, momentum m and total energy E. The fluxes for the corresponding macroscopic variables are

$$(F_\rho, F_m, F_E)^T = \int u\psi_\alpha f du d\xi. \tag{2.3}$$

The conservation principle for mass, momentum and energy during the course of particle collisions requires $Q(f,f)$ to satisfy the compatibility condition

$$\int Q(f,f)\psi_\alpha du d\xi = 0, \qquad \alpha = 1,2,3.$$

In the 1-D case, the entropy condition for the Boltzmann equation is

$$\frac{\partial H}{\partial t} + \frac{\partial G}{\partial x} \leq 0,$$

where the entropy density is

$$H = \int f \ln f du d\xi$$

and the corresponding entropy flux is

$$G = \int u f \ln f du d\xi.$$

The first-order numerical conservative scheme can be written as

$$W_j^{n+1} = W_j^n + \sigma(F_{j-1/2}^n - F_{j+1/2}^n),$$

where $W_j = (\rho_j, m_j, E_j)^T$ is the cell averaged conservative quantities, $F_{j+1/2}^n$ is the corresponding fluxes across the cell interface, and $\sigma = \Delta t/\Delta x$. For the 1st-order gas-kinetic scheme, the numerical fluxes across cell interface depend on the gas distribution function $f_{j+1/2}^n$ via (2.3). The discretized entropy condition for the above 3-point method is

$$H_j^{n+1} \leq H_j^n + \frac{\Delta t}{\Delta x}(G_{j-1/2}^n - G_{j+1/2}^n), \tag{2.4}$$

where $H_j = \int f_j \ln f_j du d\xi$ is the cell averaged entropy density and $G_{j+1/2} = \int u f_{j+1/2} \ln f_{j+1/2} du d\xi$ is the entropy flux across a cell interface. In this paper, we prove the above inequality for the KFVS scheme. Since the KFVS scheme assumes an equilibrium distribution inside cell j at the beginning of each time step, H_j^n becomes

$$\begin{aligned} H_j^n &= \int g_j^n \ln g_j^n du d\xi \\ &= \rho_j^n \ln \rho_j^n + \rho_j^n \frac{K+1}{2}(\ln \frac{\lambda_j^n}{\pi} - 1). \quad \text{(with the equilibrium distribution in Eq.(2.2))} \end{aligned} \tag{2.5}$$

Since at the beginning of each time step, the gases in the cells $j-1, j$, and $j+1$ are basically distinguishable, the updated flow variables W_j^{n+1} inside cell j at time step $n+1$ are composed of three distinguishable species from cells $j-1, j$, and $j+1$. So, the total entropy density H_j^{n+1} is the addition of the entropy of different species.

It is very difficult get a rigorous proof of the discretized entropy condition (2.4) for the nonlinear hyperbolic system. The difficulty is mostly in the interaction between numerical gas from different cells. The update of the entropy in each cell is a complicated function of all flow variables including the ones from the surrounding cells. Since the entropy condition only tells us the possible direction for a system to evolve, it does not point out exactly which way to go. So, in order to analyze the entropy condition for the discretized scheme, we design a "physical path" for the gas system to evolve. With the same initial and final conditions for the mass, momentum and energy inside each cell, the proof of the entropy condition becomes the proofs of the entropy-satisfying solution in each section of the physical path. Fortunately, for the KFVS scheme, we can design such a physical process. To show (2.4), we use results in statistical mechanics about the definition of entropy for distinguishable and indistinguishable particles.

3 KFVS Scheme

In this section we consider the kinetic flux-splitting scheme (i.e. collisionless scheme) proposed by Pullin [10] and Deshpande [2]. The scheme uses the fact that the Euler equations (2.1) are the moments of the Boltzmann equation when the velocity repartition function is Maxwellian. As numerically analyzed in [7], the flux function of the KFVS scheme is almost identical to the FVS flux of van Leer [13]. In Section 3.1 we briefly recall the collisionless scheme. In Section 3.2 we prove the entropy condition for KFVS under the standard CFL condition. The positivity of the KFVS scheme has been analyzed in [3, 9, 11].

3.1 Numerical scheme

In order to derive the collisionless Boltzmann scheme, we need to construct the numerical fluxes across each cell interface. We suppose that the initial data $(\rho(x), m(x), E(x))$ are piecewise constant over the cells $C_j = [x_{j-1/2}, x_{j+1/2}]$. At each time level, once ρ_j, m_j and E_j are given, the corresponding U_j and λ_j can be obtained by the following formulae:

$$m = \rho U, \qquad E = \frac{1}{2}\rho U^2 + \frac{K+1}{4\lambda}\rho. \tag{3.1}$$

Let

$$g_j = \rho_j \left(\frac{\lambda_j}{\pi}\right)^{\frac{K+1}{2}} e^{-\lambda_j((u-U_j)^2+\xi^2)} \tag{3.2}$$

be a Maxwellian distribution in the cell C_j. The corresponding distribution function at the cell interface is defined by

$$f(x_{j+1/2}, t, u, \xi) = \begin{cases} g_j, & \text{if } u > 0 \\ g_{j+1}, & \text{if } u < 0. \end{cases} \tag{3.3}$$

Using the formulae (2.3), we obtain the numerical fluxes

$$\begin{pmatrix} F_{\rho,j+1/2} \\ F_{m,j+1/2} \\ F_{E,j+1/2} \end{pmatrix} = \rho_j \begin{pmatrix} \frac{U_j}{2}\mathrm{erfc}(-\sqrt{\lambda_j}U_j) + \frac{1}{2}\frac{e^{-\lambda_j U_j^2}}{\sqrt{\pi\lambda_j}} \\ \left(\frac{U_j^2}{2} + \frac{1}{4\lambda_j}\right)\mathrm{erfc}(-\sqrt{\lambda_j}U_j) + \frac{U_j}{2}\frac{e^{-\lambda_j U_j^2}}{\sqrt{\pi\lambda_j}} \\ \left(\frac{U_j^3}{4} + \frac{K+3}{8\lambda_j}U_j\right)\mathrm{erfc}(-\sqrt{\lambda_j}U_j) + \left(\frac{U_j^2}{4} + \frac{K+2}{8\lambda_j}\right)\frac{e^{-\lambda_j U_j^2}}{\sqrt{\pi\lambda_j}} \end{pmatrix} \tag{3.4}$$

$$+\rho_{j+1} \begin{pmatrix} \frac{U_{j+1}}{2}\mathrm{erfc}(\sqrt{\lambda_{j+1}}U_{j+1}) - \frac{1}{2}\frac{e^{-\lambda_{j+1} U_{j+1}^2}}{\sqrt{\pi\lambda_{j+1}}} \\ \left(\frac{U_{j+1}^2}{2} + \frac{1}{4\lambda_{j+1}}\right)\mathrm{erfc}(\sqrt{\lambda_{j+1}}U_{j+1}) - \frac{U_{j+1}}{2}\frac{e^{-\lambda_{j+1} U_{j+1}^2}}{\sqrt{\pi\lambda_{j+1}}} \\ \left(\frac{U_{j+1}^3}{4} + \frac{K+3}{8\lambda_{j+1}}U_{j+1}\right)\mathrm{erfc}(\sqrt{\lambda_{j+1}}U_{j+1}) - \left(\frac{U_{j+1}^2}{4} + \frac{K+2}{8\lambda_{j+1}}\right)\frac{e^{-\lambda_{j+1} U_{j+1}^2}}{\sqrt{\pi\lambda_{j+1}}} \end{pmatrix},$$

where the complementary error function, which is a special case of the incomplete gamma function, is defined by

$$\mathrm{erfc}(x) = \frac{2}{\sqrt{\pi}}\int_x^\infty e^{-t^2}\,dt.$$

Using the above numerical fluxes, we are able to update ρ_j, m_j, E_j with the standard conservative formulations:

$$\begin{pmatrix} \tilde{\rho}_j \\ \tilde{m}_j \\ \tilde{E}_j \end{pmatrix} = \begin{pmatrix} \rho_j \\ m_j \\ E_j \end{pmatrix} + \sigma \begin{pmatrix} F_{\rho,j-1/2} - F_{\rho,j+1/2} \\ F_{m,j-1/2} - F_{m,j+1/2} \\ F_{E,j-1/2} - F_{E,j+1/2} \end{pmatrix}, \tag{3.5}$$

where $\tilde{W}_j = W_j^{n+1}$ and

$$\sigma = \frac{\Delta t}{\Delta x},$$

with Δt the stepsize in time, and Δx the mesh size in space. The scheme can be viewed as consisting of the following three steps (although it is not typically implemented this way):

ALGORITHM (KFVS Approach)

1. Given data $\{\rho_j^n, U_j^n, E_j^n\}$, compute $\{\lambda_j^n\}$ using (3.1).
2. Compute the numerical flux $\{F_{\rho,j+1/2}, F_{m,j+1/2}, F_{E,j+1/2}\}$ using (3.4).
3. Update $\{\rho_j^n, m_j^n, E_j^n\}$ using (3.5). This gives $\{\rho_j^{n+1}, m_j^{n+1}, E_j^{n+1}\}$.

3.2 Entropy analysis

The analysis of entropy condition for the KFVS scheme has attracted some attention in the past years. In [2], Deshpande stated the entropy condition in the smooth flow regions. In [5], Khobalatte and Perthame gave a proof of the maximum principle entropy condition for a gas kinetic scheme with a specific equilibrium distribution and a piecewise constant entropy function. In [8], an entropy inequality is introduced for a special distribution function. In this section, for the first time, we show that at the discretized level, the KFVS scheme satisfies the entropy condition with the exact equilibrium Maxwellian distribution.

With the same initial and final mass, momentum and energy densities in Eq.(3.5), we can design a physical path for the flow updating process. The proof of the entropy condition is based on the entropy-satisfying solution in each section of the evolving path.

In the first step, we consider the case when there is only gas flowing out from cell C_j. This gives

$$W^* = \begin{pmatrix} \rho_j^* \\ m_j^* \\ E_j^* \end{pmatrix} = \begin{pmatrix} \rho_j \\ m_j \\ E_j \end{pmatrix} + \sigma \begin{pmatrix} \int_{u<0} u g_j du d\xi - \int_{u>0} u g_j du d\xi \\ \int_{u<0} u^2 g_j du d\xi - \int_{u>0} u^2 g_j du d\xi \\ \int_{u<0} \frac{u}{2}(u^2+\xi^2) g_j du d\xi - \int_{u>0} \frac{u}{2}(u^2+\xi^2) g_j du d\xi \end{pmatrix}. \tag{3.6}$$

The second step is to consider the inflow from adjacent cell C_{j-1},

$$\hat{W} = \begin{pmatrix} \hat{\rho}_j \\ \hat{m}_j \\ \hat{E}_j \end{pmatrix} = \sigma \begin{pmatrix} \int_{u>0} u g_{j-1} du d\xi \\ \int_{u>0} u^2 g_{j-1} du d\xi \\ \int_{u>0} \frac{u}{2}(u^2+\xi^2) g_{j-1} du d\xi \end{pmatrix}. \tag{3.7}$$

In the third step, the inflow from adjacent cell C_{j+1} is considered,

$$\bar{W} = \begin{pmatrix} \bar{\rho}_j \\ \bar{m}_j \\ \bar{E}_j \end{pmatrix} = \sigma \begin{pmatrix} -\int_{u<0} u g_{j+1} du d\xi \\ -\int_{u<0} u^2 g_{j+1} du d\xi \\ -\int_{u<0} \frac{u}{2}(u^2+\xi^2) g_{j+1} du d\xi \end{pmatrix}. \tag{3.8}$$

The fourth step is to include particle collisions to let $W^*, \hat{W}$ and $\bar{W}$ in the above equations to exchange momentum and energy inside cell j and to form the individual equilibrium states $W^{*\prime}, \hat{W}'$ and $\bar{W}'$ with a common velocity and temperature,

$$\tilde{W} = \begin{pmatrix} \tilde{\rho}_j \\ \tilde{m}_j \\ \tilde{E}_j \end{pmatrix} = \begin{pmatrix} \rho_j^* \\ m_j^* \\ E_j^* \end{pmatrix} + \begin{pmatrix} \hat{\rho}_j \\ \hat{m}_j \\ \hat{E}_j \end{pmatrix} + \begin{pmatrix} \bar{\rho}_j \\ \bar{m}_j \\ \bar{E}_j \end{pmatrix} = \begin{pmatrix} \rho_j^* \\ m_j^{*\prime} \\ E_j^{*\prime} \end{pmatrix} + \begin{pmatrix} \hat{\rho}_j \\ \hat{m}_j' \\ \hat{E}_j' \end{pmatrix} + \begin{pmatrix} \bar{\rho}_j \\ \bar{m}_j' \\ \bar{E}_j' \end{pmatrix}. \tag{3.9}$$

During the above collisional phase, the individual mass, total momentum and energy are unchanged. It can be verified that $(\tilde{\rho}_j, \tilde{m}_j, \tilde{E}_j)$ obtained by (3.9) are exactly the same as those obtained by using (3.5). In terms of updating conservative variables, the above four stages form the complete KFVS scheme. The entropy density H_j^{n+1} at time $n+1$ inside cell C_j is the sum of the individual entropy of different species.

Suppose that the CFL condition

$$\sigma \leq \frac{1}{\max_j (|U_j| + c_j)} \tag{3.10}$$

is satisfied, where $c_j = \sqrt{\gamma/2\lambda_j}$ is the local speed of sound. It has been shown in [11] that the positivity conditions are precisely satisfied for the flow variables $\rho_j^* \geq 0$ and $\rho_j^* E_j^* - \frac{1}{2}(m_j^*)^2 \geq 0$, as well as $\tilde{\rho}_j \geq 0$ and $\tilde{\rho}_j \tilde{E}_j - \frac{1}{2}(\tilde{m}_j)^2 \geq 0$.

In the following, we prove that the discretized entropy condition is satisfied in the above four physical processes. As a result, the whole numerical path in the flow updating scheme satisfies the entropy condition (2.4).

Lemma 3.1 *Assume that the CFL condition is satisfied. If $\rho_j \geq 0$ and $\rho_j E_j \geq \frac{1}{2} m_j^2$, then the entropy condition is satisfied in the updating process for (ρ_j^*, m_j^*, E_j^*).*

Proof. We need to show that

$$\int_{-\infty}^{\infty} g_j^* \ln g_j^* du d\xi \leq \int_{\infty}^{\infty} g_j \ln g_j du d\xi + \sigma \left[\int_{u<0} u g_j \ln g_j du d\xi - \int_{u>0} u g_j \ln g_j du d\xi \right]. \tag{3.11}$$

We use the following relations to express the * states in terms of the j states.

$$\begin{aligned} \rho_j^* &= \rho_j - \sigma \rho_j \left\{ \frac{1}{2} U_j \alpha_j + \beta_j \right\}, \\ m_j^* &= m_j - \sigma \rho_j \left\{ \left(\frac{U_j^2}{2} + \frac{1}{4\lambda_j} \right) \alpha_j + U_j \beta_j \right\}, \\ E_j^* &= E_j - \sigma \rho_j \left\{ \left(\frac{U_j^3}{4} + \frac{K+3}{8\lambda_j} U_j \right) \alpha_j + \left(\frac{U_j^2}{2} + \frac{K+2}{4\lambda_j} \right) \beta_j \right\}, \end{aligned}$$

where

$$\alpha_j = \operatorname{erfc}\left(-\sqrt{\lambda_j} U_j\right) - \operatorname{erfc}\left(\sqrt{\lambda_j} U_j\right); \quad \beta_j = \frac{e^{-\lambda_j U_j^2}}{\sqrt{\pi \lambda_j}}. \tag{3.12}$$

The equilibrium state g_j^* has an Maxwellian distribution which corresponds to the macroscopic densities (ρ_j^*, m_j^*, E_j^*).

After some algebra,

$$\int_{-\infty}^{\infty} g_j^* \ln g_j^* du d\xi - \int_{-\infty}^{\infty} g_j \ln g_j du d\xi - \sigma \left[\int_{u<0} u g_j \ln g_j du d\xi - \int_{u>0} u g_j \ln g_j du d\xi \right] = \rho_j F,$$

where

$$\begin{aligned} F &= \left\{ \left(1 - \frac{\sigma}{2}(U_j\alpha_j + 2\beta_j)\right) \left((K+2)\ln\left(1 - \frac{\sigma}{2}(U_j\alpha_j + 2\beta_j)\right) - \frac{K+1}{2}\ln h_1 \right) - \frac{\sigma}{2}\beta_j \right\}, \\ h_1 &= 1 - \frac{\sigma\lambda_j}{K+1}(U_j\alpha_j + 2\beta_j)\left(U_j^2 + \frac{K+1}{2\lambda_j}\right) - \frac{\sigma\lambda_j}{K+1}\left(1 - \frac{\sigma}{2}(U_j\alpha_j + 2\beta_j)\right)\left\{ \left(U_j^2 + \frac{K+3}{2\lambda_j}\right) U_j\alpha_j + \right. \\ &\quad \left. \left(2U_j^2 + \frac{K+2}{\lambda_j}\right)\beta_j \right\} + \frac{2\sigma\lambda_j}{K+1}\left\{ \left(U_j^2 + \frac{1}{2\lambda_j}\right)\alpha_j U_j + 2U_j^2\beta_j \right\} - \\ &\quad \frac{2\sigma^2\lambda_j}{K+1}\left\{ \left(\frac{U_j^2}{2} + \frac{1}{4\lambda_j}\right)\alpha_j + U_j\beta_j \right\}^2 . \end{aligned}$$

The goal is to show that $F \leq 0$ for all positive σ up to the CFL limit. We can reduce the number of parameters by one by introducing the non-dimensional number $z = \sqrt{\lambda_j} U_j$ which is equivalent to the local Mach number in cell j. We also replace the parameter σ by $c \in (0,1]$ (CFL number) which is defined by:

$$\sigma = \frac{c\sqrt{\lambda_j}}{|z| + \sqrt{\gamma/2}}. \tag{3.13}$$

Let

$$\begin{aligned} \phi &= \frac{\alpha_j z}{2} + \frac{e^{-z^2}}{\sqrt{\pi}} = \mathrm{erf(z)\,z} + \frac{\mathrm{e}^{-z^2}}{\sqrt{\pi}}, \\ \psi &= \frac{e^{-2z^2}}{\pi} + z\ \mathrm{erf(z)}\frac{\mathrm{e}^{-z^2}}{\sqrt{\pi}} - \frac{\mathrm{erf(z)}^2}{2}, \\ d &= \frac{c}{|z| + \sqrt{\gamma/2}}. \end{aligned}$$

Then

$$F = (1 - d\phi)\left[\ln(1 - d\phi) - \frac{K+1}{2}\ln h\right] - \frac{e^{-z^2} d}{2\sqrt{\pi}}$$

where

$$h = 1 - \frac{d}{(K+1)(1-d\phi)^2}\left(\frac{e^{-z^2}}{\sqrt{\pi}} - d\psi\right).$$

We now proceed to show that $F = F(z, K, c) \leq 0$, where the arguments of the function are related to Mach number, gas constant, and CFL number, respectively. First note that F is an even function of z and hence we can restrict to the case $z \geq 0$. By a direct calculation, $d\phi/dz = \mathrm{erf(z)} > 0$ for $z > 0$ and thus ϕ is minimum at $z = 0$ where it equals $1/\sqrt{\pi}$. This shows that ϕ is a positive function.

Next we show that $1 - d\phi$ is positive and less than one. Since both d and ϕ are positive, it is clearly less than one. To show that it is positive, it is sufficient to show this for $c = 1$. Noting that $e^{-z^2}/\sqrt{\pi} \leq 1/\sqrt{2}$, we have

$$0 < \frac{\frac{1}{\sqrt{2}} - \frac{e^{-z^2}}{\sqrt{\pi}}}{z + \frac{1}{\sqrt{2}}} < \frac{z + \frac{1}{\sqrt{2}} - \mathrm{erf(z)z} - \frac{\mathrm{e}^{-z^2}}{\sqrt{\pi}}}{z + \frac{1}{\sqrt{2}}} \leq 1 - d\phi.$$

Now

$$\frac{e^{-z^2}}{\sqrt{\pi}} - d\psi = \frac{e^{-z^2}}{\sqrt{\pi}}\left[1 - d\left(\mathrm{erf(z)z} + \frac{\mathrm{e}^{-z^2}}{\sqrt{\pi}}\right)\right] + \frac{d}{2}\mathrm{erf(z)}^2$$
$$= \frac{e^{-z^2}}{\sqrt{\pi}}(1 - d\phi) + \frac{d}{2}\mathrm{erf(z)}^2 > 0.$$

From the above, $0 < h < 1$.

The key observation is that for any fixed K and z, F attains its maximum at $c = 0$ or $c = 1$. To show this, we explicitly compute the second derivative of F with respect to c,

$$F'' = \frac{d'^2\phi^2}{1 - d\phi} + \frac{(K+1)(1-d\phi)h'^2}{2h^2} + \frac{d'^2\mathrm{erf(z)}^2}{2h(1-d\phi)^3},$$

where $'$ denotes differentiation with respect to c. Since $F'' > 0$, F is maximum at $c = 0$ or $c = 1$ as claimed. Hence if F is negative at these values of c, then we can conclude that F is a negative function.

The first term in the Taylor series expansion of F for small c is

$$F = -d\phi + O(c^2)$$

and hence F is negative for all small c. We now restrict to the CFL limit $c = 1$.

In Figure 1, we plot F for $|z| \le 100$ and $2 \le K \le 100$. It is clear that F is a negative function.

We now examine the asymptotic behaviour of F for large values of z. For $c \in (0,1)$ and large $|z|$,

$$F = (1-c)\ln(1-c) + \frac{c}{|z|}\sqrt{\frac{\gamma}{2}}(\ln(1-c)+1) + O\left(\frac{1}{|z|^2}\right).$$

Hence $F < 0$ for large $|z|$.

In paper [11], the positivities for both $\rho_j^* \ge 0$ and $\rho_j^* E_j^* - \frac{m_j^{*2}}{2} \ge 0$ under the CFL condition have been proved. So, a distribution function f^* with $f^* \ge 0$ for the state (ρ_j^*, m_j^*, E_j^*) can be constructed.

Next we show that entropy increases in the second step where gas moves into cell C_j from its neighboring cells. It is sufficient to show only the case when gas from the left cell C_{j-1} moves into cell C_j. Denote the quantities after one time step by $(\hat{\rho}_j, \hat{m}_j, \hat{E}_j)$. See (3.7).

Before proving the entropy condition in the above process, from Jensen's inequality, it can be shown that $\hat{\rho}_j \ge 0$ and $\hat{\rho}_j\hat{E}_j - \frac{\hat{m}_j^2}{2} \ge 0$, which means that the state $(\hat{\rho}_j, \hat{m}_j, \hat{E}_j)$ satisfies the positivity condition. So, a gas distribution function $\hat{f}$ with $\hat{f} \ge 0$ can also be obtained from this state.

Lemma 3.2 *Assume that $\hat{\rho}_j, \hat{m}_j, \hat{E}_j$ are computed by (3.7). With the CFL condition, the entropy condition is satisfied in the process to obtain $(\hat{\rho}_j, \hat{m}_j, \hat{E}_j)$.*

Proof. After some algebra, we have

$$\int_{-\infty}^{\infty} \hat{g}_j \ln \hat{g}_j du d\xi - \sigma \int_{u>0} u g_{j-1} \ln g_{j-1} du d\xi = \frac{1}{2}\rho_{j-1}\frac{c}{|z| + \sqrt{\gamma/2}}F,$$

where

$$F = \phi\left[\ln\left(\frac{c\phi}{2(|z| + \sqrt{\gamma/2})}\right) + (K+1)\ln\frac{\phi}{\sqrt{\phi^2 + \frac{\psi}{K+1}}}\right] + \frac{e^{-z^2}}{2\sqrt{\pi}},$$

$$\phi = z\ \mathrm{erfc}(-z) + \frac{e^{-z^2}}{\sqrt{\pi}},$$

$$\psi = \frac{e^{-2z^2}}{\pi} + z\ \mathrm{erfc}(-z)\frac{e^{-z^2}}{\sqrt{\pi}} - \frac{\mathrm{erfc}(-z)^2}{2}.$$

The goal is to show that the entropy condition is satisfied or equivalently, $F(z, K, c) \leq 0$. As previously, we have introduced the non-dimensional number $z = \sqrt{\lambda_{j-1}}U_{j-1}$ and the number c is as defined in (3.13) but with j changed to $j-1$. First note that $\phi > 0$ for all real values of z. To show this, note that $d\phi/dz = \mathrm{erfc}(-z) > 0$ and thus the minimum of ϕ occurs at $z = -\infty$ where $\phi = 0$. Hence it is apparent that among the possible values of $c \in (0, 1]$, F is maximum at $c = 1$. Thus it is sufficient to demonstrate that $F \leq 0$ for $c = 1$. We shall assume this value of c for the remainder of this proof so that F is now a function of K and z.

It can be shown that ψ is negative for all z. Now for a fixed z, the term

$$\ln\left(\frac{\phi}{2(|z| + \sqrt{\gamma/2})}\right)$$

in F is maximum when $\gamma = 1$ or $K = \infty$. The second term

$$(K+1)\ln\left(\frac{\phi}{\sqrt{\phi^2 + \frac{\psi}{K+1}}}\right)$$

is a decreasing function of K. This can be shown by taking its derivative with respect to K and it is

$$D = -\frac{1}{2}\ln(1+y) + \frac{1}{2}\frac{y}{1+y},$$

where

$$y = \frac{\psi}{(K+1)\phi^2}.$$

Note that $-1 < y < 0$. The derivative D can be shown to be negative for all $y \in (-1, 0)$. Thus the second term achieves its maximum at $K = 2$. Hence we conclude that

$$F < \phi\left[\ln\left(\frac{\phi}{2(|z| + \sqrt{.5})}\right) - \frac{3}{2}\ln\left(1 + \frac{\psi}{3\phi^2}\right)\right] + \frac{e^{-z^2}}{2\sqrt{\pi}} \equiv G(z).$$

For $z \in (0, \infty)$, $G_z < 0$ and since $G(0) = -.5775\cdots$, we have shown that $G < 0$ on $[0, \infty)$. For $z < 0$, G is maximum at $z = -\infty$. As $z \to -\infty$, the first term of the asymptotic expansion of G is

$$G \approx -\frac{3e^{-z^2}\ln|z|}{2\sqrt{\pi}z^2}$$

and so it is a negative function for $z < 0$. Thus we conclude that F is negative and thus the entropy condition is satisfied. We have finished the proof of the lemma.

We plot $F(z, K)$ in Figure 2.

As a result, we have

$$\int_{-\infty}^{\infty} \hat{g}_j \ln \hat{g}_j du d\xi \leq \sigma \int_{u>0} u g_{j-1} \ln g_{j-1} du d\xi. \tag{3.14}$$

Similarly, we have

$$\int_{-\infty}^{\infty} \bar{g}_j \ln \bar{g}_j du d\xi \leq -\sigma \int_{u<0} u g_{j+1} \ln g_{j+1} du d\xi. \tag{3.15}$$

for the particles coming from the cell $j+1$ on the right hand side.

After all terms of (ρ^*, m^*, E^*), $(\hat{\rho}, \hat{m}, \hat{E})$, $(\bar{\rho}, \bar{m}, \bar{E})$ are obtained, the flow variables in each cell C_j are updated according to Eq.(3.9). Since positivity is satisfied for each species (ρ^*, m^*, E^*), $(\hat{\rho}, \hat{m}, \hat{E})$ and $(\bar{\rho}, \bar{m}, \bar{E})$, the distribution functions $g^*, \hat{g}, \bar{g}$ satisfy the conditions $g^* \geq 0, \hat{g} \geq 0, \bar{g} \geq 0$. In the collisional step, different species with its individual identification $W^*, \hat{W}$ and $\bar{W}$ are mixed to form equilibrium states $g^{*\prime}, \hat{g}'$ and $\bar{g}'$ with a common velocity U and temperature λ. In the collisional process, the individual mass, total momentum and energy are conserved, and the individual equilibrium states become

$$\begin{aligned} g^{*\prime} &= \rho^* \left(\frac{\lambda}{\pi}\right)^{\frac{K+1}{2}} e^{-\lambda((u-U)^2+\xi^2)}, \\ \hat{g}' &= \hat{\rho} \left(\frac{\lambda}{\pi}\right)^{\frac{K+1}{2}} e^{-\lambda((u-U)^2+\xi^2)}, \\ \bar{g}' &= \bar{\rho} \left(\frac{\lambda}{\pi}\right)^{\frac{K+1}{2}} e^{-\lambda((u-U)^2+\xi^2)}, \end{aligned} \tag{3.16}$$

where λ and U are determined from the total momentum and energy conservations Eq.(3.9),

$$(\rho^* + \hat{\rho} + \bar{\rho})U = m^* + \hat{m} + \bar{m}$$

and

$$(\rho^* + \hat{\rho} + \bar{\rho})(\frac{1}{2}U^2 + \frac{K+1}{4\lambda}) = E^* + \hat{E} + \bar{E}.$$

Lemma 3.3 *The collision stage from $(g^*, \hat{g}, \bar{g})$ to $(g^{*\prime}, \hat{g}', \bar{g}')$ satisfies the entropy condition.*

Proof. Since

$$g^* \geq 0 \quad , \quad \hat{g} \geq 0 \quad , \quad \bar{g} \geq 0,$$

and the individual mass, total momentum and energy conservations are satisfied, we have

$$\begin{aligned} &\int g^{*\prime} \ln g^{*\prime} du d\xi + \int \hat{g}' \ln \hat{g}' du d\xi + \int \bar{g}' \ln \bar{g}' du d\xi - \int g^* \ln g^* du d\xi - \int \hat{g} \ln \hat{g} du d\xi - \int \bar{g} \ln \bar{g} du d\xi \\ &= \int (g^{*\prime} - g^*) \ln g^{*\prime} du d\xi + \int g^* \ln(g^{*\prime}/g^*) du d\xi + \int (\hat{g}' - \hat{g}) \ln \hat{g}' du d\xi + \int \hat{g} \ln(\hat{g}'/\hat{g}) du d\xi \\ &\quad + \int (\bar{g}' - \bar{g}) \ln \bar{g}' du d\xi + \int \bar{g} \ln(\bar{g}'/\bar{g}) du d\xi \\ &= \int g^* \ln(g^{*\prime}/g^*) du d\xi + \int \hat{g} \ln(\hat{g}'/\hat{g}) du d\xi + \int \bar{g} \ln(\bar{g}'/\bar{g}) du d\xi \\ &\leq \int g^*(g^{*\prime}/g^* - 1) du d\xi + \int \hat{g}(\hat{g}'/\hat{g} - 1) du d\xi + \int \bar{g}(\bar{g}'/\bar{g} - 1) du d\xi \\ &= \int (g^{*\prime} - g^*) du d\xi + \int (\hat{g}' - \hat{g}) du d\xi + \int (\bar{g}' - \bar{g}) du d\xi \\ &= 0. \end{aligned}$$

In conclusion, we have

$$\int g^{*\prime} \ln g^{*\prime} du d\xi + \int \hat{g}' \ln \hat{g}' du d\xi + \int \bar{g}' \ln \bar{g}' du d\xi \leq \int g^* \ln g^* du d\xi + \int \hat{g} \ln \hat{g} du d\xi + \int \bar{g} \ln \bar{g} du d\xi. \quad (3.17)$$

Once we have $g^{*\prime}, \hat{g}'$ and $\bar{g}'$, the total entropy of the distinguishable particle system inside cell C_j is

$$H' = \int g^{*\prime} \ln g^{*\prime} du d\xi + \int \hat{g}' \ln \hat{g}' du d\xi + \int \bar{g}' \ln \bar{g}' du d\xi, \quad (3.18)$$

and the total distribution function is

$$\begin{aligned} g &= g^{*\prime} + \hat{g}' + \bar{g}' \\ &= \rho^* \left(\frac{\lambda}{\pi}\right)^{\frac{K+1}{2}} e^{-\lambda((u-U)^2+\xi^2)} + \hat{\rho} \left(\frac{\lambda}{\pi}\right)^{\frac{K+1}{2}} e^{-\lambda((u-U)^2+\xi^2)} + + \bar{\rho} \left(\frac{\lambda}{\pi}\right)^{\frac{K+1}{2}} e^{-\lambda((u-U)^2+\xi^2)} \quad (3.19) \\ &= (\rho^* + \hat{\rho} + \bar{\rho}) \left(\frac{\lambda}{\pi}\right)^{\frac{K+1}{2}} e^{-\lambda((u-U)^2+\xi^2)}. \end{aligned}$$

With the updated $(\tilde{\rho}, \tilde{m}, \tilde{E})$ inside cell C_j in Eq.(3.9), the total entropy H_j^{n+1} is composed of the sum of the individual entropies of three species,

$$\begin{aligned} H_j^{n+1} &= H' \\ &= \int g^{*\prime} \ln g^{*\prime} du d\xi + \int \hat{g}' \ln \hat{g}' du d\xi + \int \bar{g}' \ln \bar{g}' du d\xi \\ &= \rho^* \ln \rho^* + \rho^* \frac{K+1}{2}(\ln \frac{\lambda}{\pi} - 1) + \hat{\rho} \ln \hat{\rho} + \hat{\rho} \frac{K+1}{2}(\ln \frac{\lambda}{\pi} - 1) + \bar{\rho} \ln \bar{\rho} + \bar{\rho} \frac{K+1}{2}(\ln \frac{\lambda}{\pi} - 1). \quad (3.20) \end{aligned}$$

With the Lemma(3.1-3.3) and the total entropy of three species at step $n+1$, we have

Theorem 3.1 *The entropy condition (2.4) is satisfied in the KFVS scheme.*

Proof. From Equations (3.11), (3.14), (3.15), (3.17), and (3.19), the new total entropy for the three species at cell j is

$$\begin{aligned} H_j^{n+1} &= H' \\ &= \int g^{*\prime} \ln g^{*\prime} du d\xi + \int \hat{g}' \ln \hat{g}' du d\xi + \int \bar{g}' \ln \bar{g}' du d\xi \\ &\leq \int g^* \ln g^* du d\xi + \int \hat{g} \ln \hat{g} du d\xi + \int \bar{g} \ln \bar{g} du d\xi \quad \text{(Lemma 3.3)} \\ &\leq H_j^n + \frac{\Delta t}{\Delta x}(G_{j-1/2}^n - G_{j+1/2}^n). \quad \text{(Add Eqns.(3.11), (3.14) and (3.15))} \end{aligned}$$

Remark: the flow variables W_j^{n+1} inside cell j at $n+1$ do consist of three distinguishable species.

For any numerical scheme, basically we are only remembering the conservative quantities inside each cell and the entropy is a function of the conservative variables. However, beside this, the entropy concept is also related to the information. For example, the entropy is different for a gas composed of one single color and a gas composed of two different colors. Numerically, at the beginning of each time step, we divide the gas into different cells. Consequently, the gases in different cells become distinguishable. For example, ρ_{j-1}^n can be regarded as blue, ρ_j^n as yellow and ρ_{j+1}^n as red. As a result, inside cell C_j at the end of time step $n+1$, the gas ρ_j^{n+1} is composed of three species, i.e., red, yellow and blue, and the entropy H_j^{n+1} is the sum of the entropies of the individual species. The distinguishable effect of particles is purely due to numerical artifacts such as discretized space but they have a physical consequence. In order to remove the numerical effect at time step $n+1$ inside cell C_j, we can numerically erase the different "colors" of the gas. More precisely, we can remove the individual history of the gas inside cell C_j. As a result, the total density $\tilde{\rho}$ CANNOT keep the information of the individual densities $(\rho^*, \hat{\rho}, \bar{\rho})$, and the equilibrium state Eq.(3.19) goes to

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

The corresponding entropy becomes

$$\begin{aligned} H &= \int \tilde{g} \ln \tilde{g} du d\xi \\ &= \tilde{\rho} \ln \tilde{\rho} + \tilde{\rho}\frac{K+1}{2}(\ln \frac{\lambda}{\pi} - 1). \end{aligned} \tag{3.21}$$

Note that for the same number of particles inside cell j at time $n+1$, there is quantitative differences in the entropies between distinguishable (Eq.(3.20)) and indistinguishable (Eq.(3.21)) system. This phenomena is related to the so-called Gibbs paradox [12].

The above post-process has no direct dynamical effect on the KFVS scheme in the updating of conservative variables, and has no effect on the proof of the entropy condition in this paper. We are perfectly allowed to keep the individual species inside cell j at time $n+1$, and there is no need to take the above post-process to erase different colors and make them indistinguishable in terms of the updating conservative variables.

4 Conclusion

The gas-kinetic scheme provides an approximate Riemann solution for the Euler equations. The entropy condition for the Kinetic Flux Vector Splitting is proved in this paper. Based on the positivity and entropy analysis, we can conclude that the KFVS is one of the most robust schemes for CFD applications.

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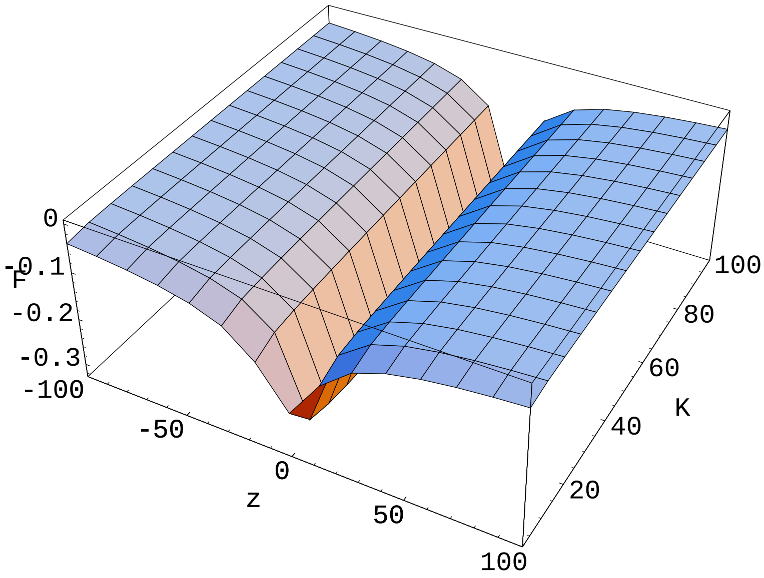

Figure 1: Plot of $F(z, K)$ at $c = 1$.

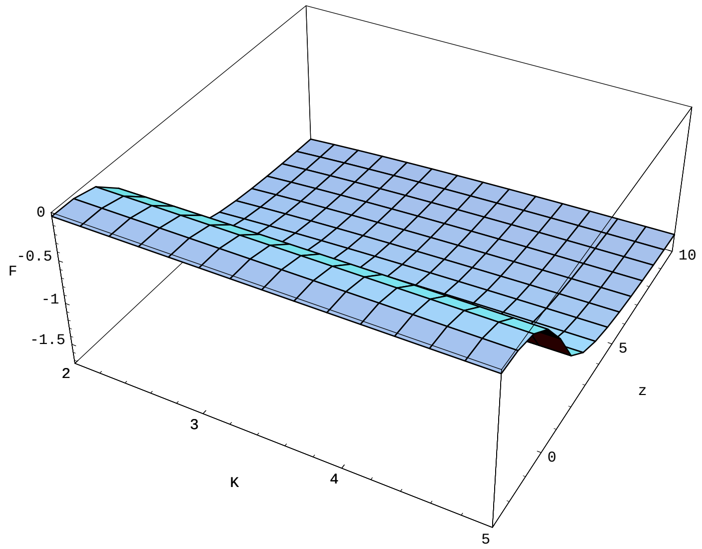

Figure 2: Plot of $F(z, K)$.