4.Volumetric Lattice Boltzmann Models in General Curvature

Chen Peng Chung

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Contents

1 Gauss-Hermit quadrature rule

This section shows the process of extending the 1-dimensional n-order Gauss-Hermite quadrature to the 3-dimensional n-order Gauss-Hermite quadrature rule. The equation below is the basic quadrature rule for evaluating integrals.

$$\int_{-\infty}^{\infty} dr\omega(r)\mathrm{P}^{2n-1}(r) = \sum_{i=1}^{n} w_i \mathrm{P}^{2n-1}(r_i) \tag{1.1}$$

The equation above is the one-dimensional n-order Gauss-Hermite quadrature rule, where the function P^{2n-1} is any (2n-1)-order polynomial, so the rule applies to any (2n-1)-order polynomial. The one-dimensional n-order Gauss-Hermite quadrature rule can be extended to any function whose order is smaller than 2n-1. The list below provides the information needed to explain the equation above.

Generation function	$\omega(r)$	$\frac{1}{\sqrt{2\pi}} \exp\left(-\frac{r^2}{2}\right)$
Nodes	r_i	The roots of 1 dimension n orders Hermite polynomial $\mathrm{H}^{(n)}(r)$
Weights	w_i	$\frac{n!}{\left(n\mathrm{H}^{(n-1)}(r)\right)^2}$

The generation function of one dimension n orders Hermite polynomial is $\omega(x)$, and weight function of 3 dimensions n orders Hermite polynomial is $\omega(\vec{r})$.

$$\begin{aligned} \omega(x) &= \frac{1}{\sqrt{2\pi}} e^{\frac{-x^2}{2}} \\ \omega(\vec{r}) &= \frac{1}{\sqrt{2\pi}} e^{\frac{-\vec{r}\cdot\vec{r}}{2}} \end{aligned} \tag{1.2}$$

The variables r_i are the roots of the one-dimensional n-order Hermite polynomial. Note that an n-order Hermite polynomial has n roots, i.e., the order is equal to the number of roots.

3-dimensional n-order Hermite polynomials The definition of the 3-dimensional n-order Hermite polynomials is given below:

$$\overleftrightarrow{H}^{(n)}(\vec{r}) \equiv (-1)^n \frac{1}{\omega(\vec{r})} \vec{\nabla}^{(n)} \omega(\vec{r}) \tag{1.3}$$

The symbol $\vec{\nabla}$ denotes the gradient of the weight function. An n-order Hermite polynomial is an n-order tensor field. The order of the tensor field is equal to the number of gradient operators in the Hermite formula. For example, the 2-dimensional second-order Hermite polynomial:

$$\begin{aligned} \overleftrightarrow{H}^{(2)}(x,y) &= H_{xx}^{(2)} \vec{e}_x \vec{e}_x + H_{xy}^{(2)} \vec{e}_x \vec{e}_y + H_{yy}^{(2)} \vec{e}_y \vec{e}_y \\ &= \left(x^2 - 1\right) \vec{e}_x \vec{e}_x + xy\, \vec{e}_x \vec{e}_y + \left(y^2 - 1\right) \vec{e}_y \vec{e}_y \end{aligned} \tag{1.4}$$

For any $(2n-1)$-order polynomial, the one-dimensional n-order Gauss-Hermite quadrature rule can evaluate the integral whose domain is $-\infty$ to ∞ .

Gauss-Hermite promoted to high dimensions Consider a volume integration over the whole three-dimensional space:

$$\int_\Omega d^3r\omega(\vec{r})\mathrm{P}^{\mathrm{N}}(\vec{r}) = \int_\Omega d^3r\omega(\vec{r}) \sum_{a+b+c\leq N} x^a y^b z^c \tag{1.5}$$

Because the summation has a finite number of terms, the integration can be moved into the summation. We have

$$\sum_{a+b+c\leq N} \int_\Omega d^3r\omega(\vec{r}) x^a y^b z^c \tag{1.6}$$

Now we use the property of the exponential function:

$$\omega(\vec{r}) = \omega(x)\omega(y)\omega(z)$$

$$\sum_{a+b+c\leq N} \int_\Omega d^3r\omega(\vec{r}) x^a y^b z^c = \sum_{a+b+c\leq N} \int_\Omega dx\omega(x)x^a \int_\Omega dy\omega(y)y^b \int_\Omega dz\omega(z)z^c \tag{1.7}$$

Using the one-dimensional n-order Gauss-Hermite quadrature rule for each integration along different directions, we have

$$\sum_{a+b+c\leq N} \sum_{i=1}^{n_a} \omega(x_i)x_i^a \sum_{i=1}^{n_b} \omega(y_i)y_i^b \sum_{i=1}^{n_c} \omega(z_i)z_i^c \tag{1.8}$$

where $(2n_a - 1) > a$, $(2n_b - 1) > b$, $(2n_c - 1) > c$. The details are as follows:

$$\int_\Omega dx\omega(x)x^a = \sum_{i=1}^{n_a} \omega(x_i)x_i^a \text{ (1 dimension } n_a \text{ order G-H rule)} \tag{1.9}$$

where x_i is the root of the one-dimensional n_a-order Hermite function. Usually, for each one-dimensional Gauss-Hermite quadrature rule, we take the order to match the integrated function, i.e., the maximum order among the polynomial terms, so we can take the summation to handle the integration above:

$$\sum_{a+b+c\leq N} \int_\Omega d^3r\omega(\vec{r}) x^a y^b z^c = \sum \sum_{i=1}^{(N-1)/2} \omega(x_i)x_i^a \sum_{i=1}^{(N-1)/2} \omega(y_i)y_i^b \sum_{i=1}^{(N-1)/2} \omega(z_i)z_i^c \tag{1.10}$$

For example, calculate the integral $\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy\omega(x,y)x^2y$

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy\omega(x,y)x^2y = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy\frac{1}{\sqrt{2\pi}}e^{\frac{-(x^2+y^2)}{2}}x^2y = (w_1y_1 + w_2y_2)\left(w_1x_1^2 + w_2x_2^2\right)$$

2 Momentum Loss of Distribution Function in Propagation

In general curvilinear coordinates, macroscopic values (i.e., ρ, $\rho\vec{u}$) experience losses due to curvature and nonuniform properties. This paper shows the value below:

$$\delta N_\alpha(\vec{q},t) \equiv N_\alpha(\vec{q},t) - N_\alpha^\star(\vec{q} - \vec{e}_\alpha\delta t, t-1) \tag{2.1}$$

where q is the nondimensional position, and its original form is $\vec{q} = (q_1, q_2, q_3)$. The value $N^\star$ represents post-collision distribution function. We can review the Lattice Boltzmann Equation-BGK

(LBGK) and see where the term appears in the equation.

$$N_\alpha(\vec{q}+\vec{e}_\alpha\delta t, t+1) = N_\alpha(\vec{q},t) + \Omega_\alpha + \delta N_\alpha(\vec{q},t) \tag{2.2}$$

For general orthogonal curvilinear coordinates in three dimensions, the loss of momentum and the loss of density are 0, so we have the relation:

$$\sum_{\alpha=0}^{q-1} \delta N_\alpha(\vec{q},t) = \sum_{\alpha=0}^{q-1} N_\alpha(\vec{q},t) - N_\alpha^\star(\vec{q}-\vec{e}_\alpha\delta t, t-1) = \sum_{\alpha=0}^{q-1} N_\alpha(\vec{q},t) - \sum_{\alpha=0}^{q-1} N_\alpha^\star(\vec{q}-\vec{e}_\alpha\delta t, t-1) = 0 \tag{2.3}$$

But for momentum loss, we first consider its physical meaning as an "inertial force." The value in equation (2.1) is a modified term in the process of the streaming step. The reason why we have to consider the loss is to achieve momentum conservation by adding this term.

Definition 2.1.

$$\vec{\Theta}_i^j(\vec{q}+\vec{e}_\alpha\delta t, \vec{q}) = [\vec{g}_i(\vec{q}+\vec{e}_\alpha\delta t) - \vec{g}_i(\vec{q})] \cdot \vec{g}^{\,j}(\vec{q}) \tag{2.4}$$

We call this value the "nondimensional change of curvature tangent vector," where $\vec{g}^j$ can be defined as below:

$$\vec{g}^1 = \frac{\vec{g}_2 \times \vec{g}_3}{(\vec{g}_2 \times \vec{g}_3)\cdot \vec{g}_1} \tag{2.5}$$

Substituting the vector into equation (2.4)

$$\vec{\Theta}_i^j(\vec{q}+\vec{e}_\alpha\delta t, \vec{q}) = [\vec{g}_i(\vec{q}+\vec{e}_\alpha\delta t) - \vec{g}_i(\vec{q})] \cdot \frac{\vec{g}_2 \times \vec{g}_3}{(\vec{g}_2 \times \vec{g}_3)\cdot \vec{g}_1} \tag{2.6}$$

Definition 2.2.

$$\begin{aligned}
\vec{M}_{\text{Loss}}(\vec{q},t) &\equiv \sum_{\alpha=1}^{q} [N_\alpha(\vec{q},t)\,\vec{e}_\alpha(\vec{q}) - N_\alpha^\star(\vec{q}-\vec{e}_\alpha\delta t, t-1)\,\vec{e}_\alpha(\vec{q}-\vec{e}_\alpha\delta t)] \\
\vec{M}_{\text{Loss}}(\vec{q}+\vec{e}_\alpha\delta t, t+1) &\equiv \sum_{\alpha=1}^{q} [N_\alpha(\vec{q}+\vec{e}_\alpha\delta t, t+1)\,\vec{e}_\alpha(\vec{q}+\vec{e}_\alpha\delta t) - N_\alpha^\star(\vec{q},t)\,\vec{e}_\alpha(\vec{q})]
\end{aligned} \tag{2.7}$$

For curvilinear coordinates, the loss of momentum always exists in the streaming step. The basic reason for the loss of macroscopic value is:

$$N_\alpha(\vec{q},t) \neq N_\alpha^\star(\vec{q}-\vec{e}_\alpha\delta t, t-1) \tag{2.8}$$

The pre-streaming distribution function is different from the post-collision function, but the sum of distributions along the discrete velocity space is the same for the two function sets. We can see that density cannot be lost in the streaming step in curvilinear coordinates. But this paper defines two values for inner and outer momentum loss at the point (q,t), as shown, to prepare for proving the inertial force.

Definition 2.3.

$$\begin{aligned}\mathcal{J}(\vec{q})\,\vec{\chi}^{\text{in}}(\vec{q},t) &\equiv -\sum_{\alpha=1}^{q} N_\alpha(\vec{q},t)\cdot(\vec{e}_\alpha(\vec{q})-\vec{e}_\alpha(\vec{q}-\vec{e}_\alpha\delta t))\\ \mathcal{J}(\vec{q})\,\vec{\chi}^{\text{out}}(\vec{q},t) &\equiv -\sum_{\alpha=1}^{q}(\vec{e}_\alpha(\vec{q}+\vec{e}_\alpha\delta t)-\vec{e}_\alpha(\vec{q}))\cdot N^\star_\alpha(\vec{q},t)\end{aligned} \tag{2.9}$$

where for the discrete particle velocity set

$$\vec{\tilde{c}}_\alpha(\vec{q})=\vec{e}_\alpha(\vec{q})=\sum_{i=1}^{3}(\vec{c}_\alpha\cdot\vec{g}_i)\frac{\Delta x}{\Delta t}=c^i_\alpha\,\vec{g}_i\,\frac{\Delta x}{\Delta t} \tag{2.10}$$

In this paper, the momentum loss and its definition can be separated into two directions at the point $(\vec{q},t)$, i.e., inner and outer. The difference from the true ”momentum loss of the propagation” is that it takes the post-collision distribution function at $(\vec{q}-\vec{e}_\alpha\delta t,t-1)$: $N^\star_\alpha(\vec{q}-\vec{e}_\alpha\delta t,t-1)$; and it takes the pre-collision function at $(\vec{q},t)$: $N_\alpha(\vec{q},t)$ for the curvilinear normalized discrete particle velocity set: $\vec{\tilde{e}}_\alpha(\vec{q}-\vec{e}_\alpha\delta t,t-1)$ and $\vec{\tilde{e}}_\alpha(\vec{q},t)$. The author takes the constraint for momentum in the process of propagation as shown:

$$\begin{aligned}&\sum_{\alpha=1}^{q}\vec{e}_\alpha(\vec{q},t)\,\delta N_\alpha(\vec{q})=\sum_{\alpha=1}^{q}\vec{e}_\alpha(\vec{q})\,N_\alpha(\vec{q})-\sum_{\alpha=1}^{q}\vec{e}_\alpha(\vec{q})\,N^\star_\alpha(\vec{q}-\vec{e}_\alpha\delta t,t-1)=\mathcal{J}\cdot\frac{\vec{\chi}^{\text{in}}(\vec{q},t)+\vec{\chi}^{\text{out}}(\vec{q},t)}{2}\\ &=\mathcal{J}\cdot\frac{-\sum_{\alpha=1}^{q}N_\alpha(\vec{q})\,(\vec{e}_\alpha(\vec{q})-\vec{e}_\alpha(\vec{q}-\vec{e}_\alpha\delta t))-\sum_{\alpha=1}^{q}N^\star_\alpha(\vec{q},t)\,(\vec{e}_\alpha(\vec{q}+\vec{e}_\alpha\delta t)-\vec{e}_\alpha(\vec{q}))}{2}\end{aligned} \tag{2.11}$$

Definition 2.4. Velocity-space discretized force field – specific case in curvilinear coordinates

$$F^i(\vec{q},t)=\frac{\vec{\chi}^{\text{in}}(\vec{q},t)+\vec{\chi}^{\text{out}}(\vec{q},t)}{2}\cdot\vec{g}^{\,i}(\vec{q}) \tag{2.12}$$

The macroscopic force is discretized in particle-velocity space, and this represents an inertial force produced in a curvilinear-coordinate computational domain. We now review the statement of the whole process. First, we impose two ”symbols” for inner and outer momentum loss; then define the form of the velocity space-discretized force field, and finally prove the inertial force using the momentum loss. However, the following expression appears to treat a symbol as a ”variable”:

$$\left(\sum_{\alpha=1}^{q}(\vec{e}_\alpha(\vec{q})-\vec{e}_\alpha(\vec{q}-\vec{e}_\alpha\delta t))\cdot N_\alpha(\vec{q},t)\right)$$

which is not exactly the momentum loss. The author then uses the true constraint to define the inertial force and maps that constraint to a velocity-space discretized force field. The specific issues are:

1. The definition of any force (including a velocity-discrete force field) should take a form like

$$\begin{aligned}F^i(\vec{q},t)&\equiv\frac{\text{Momentum Loss}}{\Delta t}\cdot\vec{e}_i\ \text{(gerneral definition)}\\ \mathcal{J}(\vec{q})F^i(\vec{q},t)&\equiv\frac{\text{Momentum Loss}}{\Delta t}\cdot\vec{e}_i\frac{1}{|\vec{g}_i|}\end{aligned} \tag{2.13}$$

where $\hat{g}_i = \dfrac{\vec{g}_i}{|\vec{g}_i|}$ is the unit vector in the i-th coordinate direction. This form uses a time difference (division by Δt) and projects onto the unit vector to obtain the component. The author's original expression omits the time scaling and the projection, which complicates interpretation. I thought that he set the time step is 1.

2. The second issue concerns the use of $\vec{g}^{\,i}$ in equation (2.12). If $\vec{g}^{\,i}$ is intended to extract a component, it should be the unit vector $\hat{g}^{\,i}$. Multiplying by the magnitude $|\vec{g}^{\,i}|$ changes the scaling and can remove the proper coordinate-transformation property of the discrete force field. If a Jacobian or metric factor is required, it should be introduced explicitly and justified.

Derivation. Derivation of the equation

$$\mathcal{J}(\vec{q})F^{\,i}(\vec{q},t) = \frac{-1}{2}\Big(\sum_{\alpha=1}^{q} N_\alpha(\vec{q},t)\left(c_\alpha^i \Theta_i^j(\vec{q}-\vec{e}_\alpha \delta t,\vec{q})\right) + \sum_{\alpha=1}^{q} N_\alpha^\star(\vec{q},t)\left(c_\alpha^i \Theta_i^j(\vec{q}+\vec{e}_\alpha \delta t,\vec{q})\right) \tag{2.14}$$

The principle of the derivation can be separated into three parts:

1. $\sum_{\alpha=1}^{q} \vec{e}_\alpha(\vec{q})\,\delta N_\alpha(\vec{q},t) \equiv$ Momentum Loss of the Streaming Step
2. $\sum_{\alpha=1}^{q} \vec{e}_\alpha(\vec{q})\,\delta N_\alpha(\vec{q},t) \equiv \mathcal{J}(\vec{q})\cdot\frac{\vec{\chi}^{\,in}+\vec{\chi}^{\,out}}{2}$ (for Volumetric LBM)
3. Velocity space discretized force field $\mathcal{J}(\vec{q})F^{\,i} \equiv \frac{\text{Momentum Loss}}{\Delta t}\cdot\vec{e}_j\frac{1}{|\vec{g}_j|}$

$$\mathcal{J}(\vec{q})F^1 = \sum_{\alpha=1}^{q}\vec{e}_\alpha(\vec{q})\delta N_\alpha(\vec{q},t)\cdot\vec{g}^{\,1} = \sum_{\alpha=1}^{q}\vec{e}_\alpha(\vec{q})\delta N_\alpha(\vec{q},t)\cdot\frac{\vec{g}_2\times\vec{g}_3}{(\vec{g}_2\times\vec{g}_3)\cdot\vec{g}_1}$$

$$= \frac{-1}{2}\left(\sum_{\alpha=1}^{q} N_\alpha(\vec{q},t)\left(\vec{e}_\alpha(\vec{q})-\vec{e}_\alpha(\vec{q}-\vec{e}_\alpha\delta t)\right) + \sum_{\alpha=1}^{q} N_\alpha^\star(\vec{q},t)\left(\vec{e}_\alpha(\vec{q}+\vec{e}_\alpha\delta t)-\vec{e}_\alpha(\vec{q})\right)\right)\cdot\frac{\vec{g}_2\times\vec{g}_3}{(\vec{g}_2\times\vec{g}_3)\cdot\vec{g}_1}$$

$$= \sum_{\alpha=1}^{q}\vec{e}_\alpha(\vec{q})\delta N_\alpha(\vec{q},t)\cdot\vec{e}_j\frac{1}{|\vec{g}_j|}$$

$$= \frac{-1}{2}\left(\sum_{\alpha=1}^{q} N_\alpha(\vec{q},t)\left(\vec{e}_\alpha(\vec{q})-\vec{e}_\alpha(\vec{q}-\vec{e}_\alpha\delta t)\right) + \sum_{\alpha=1}^{q} N_\alpha^\star(\vec{q},t)\left(\vec{e}_\alpha(\vec{q}+\vec{e}_\alpha\delta t)-\vec{e}_\alpha(\vec{q})\right)\right)\cdot\vec{e}_j\frac{1}{|\vec{g}_j|}$$

$$= \frac{-1}{2}\Big(\sum_{\alpha=1}^{q} N_\alpha(\vec{q},t)\left(\vec{e}_\alpha(\vec{q})\cdot\vec{e}_j\frac{1}{|\vec{g}_j|} - \vec{e}_\alpha(\vec{q}-\vec{e}_\alpha\delta t)\cdot\vec{e}_j\frac{1}{|\vec{g}_j|}\right)$$

$$+ \sum_{\alpha=1}^{q} N_\alpha^\star(\vec{q},t)\left(\vec{e}_\alpha(\vec{q}+\vec{e}_\alpha\delta t)\cdot\vec{e}_j\frac{1}{|\vec{g}_j|} - \vec{e}_\alpha(\vec{q})\cdot\vec{e}_j\frac{1}{|\vec{g}_j|}\right)\Big)$$

$$= \frac{-1}{2}\left(\sum_{\alpha=1}^{q} N_\alpha(\vec{q},t)\left(c_\alpha^j\cdot\frac{|\vec{g}_j|(\vec{q})-|\vec{g}_j|(\vec{q}-\vec{e}_\alpha\delta t))}{|\vec{g}_j|}\right) + \sum_{\alpha=1}^{q} N_\alpha^\star(\vec{q},t)\left(c_\alpha^j\cdot\frac{|\vec{g}_j|(\vec{q}+\vec{e}_\alpha\delta t)-|\vec{g}_j|(\vec{q}))}{|\vec{g}_j|}\right)\right)$$

$$= \frac{-1}{2}\left(\sum_{\alpha=1}^{q} N_\alpha(\vec{q},t)\left(c_\alpha^j\cdot\frac{|\vec{g}_j|(\vec{q}-\vec{e}_\alpha\delta t)-|\vec{g}_j|(\vec{q})}{|\vec{g}_j|}\right) + \sum_{\alpha=1}^{q} N_\alpha^\star(\vec{q},t)\left(c_\alpha^j\cdot\frac{|\vec{g}_j|(\vec{q}+\vec{e}_\alpha\delta t)-|\vec{g}_j|(\vec{q}))}{|\vec{g}_j|}\right)\right) \tag{2.15}$$

$$= \frac{-1}{2}\left(\sum_{\alpha=1}^{q} N_\alpha(\vec{q},t)\left(c_\alpha^i \Theta_i^j(\vec{q}-\vec{e}_\alpha\delta t,\vec{q})\right) + \sum_{\alpha=1}^{q} N_\alpha^\star(\vec{q},t)\left(c_\alpha^i \Theta_i^j(\vec{q}+\vec{e}_\alpha\delta t,\vec{q})\right)\right) \tag{2.16}$$

2.1 Basic Equation for Curvilinear Coordinate

These are basic formula for standard Latticve Boltzmann Method to achieve conservation, we can use them to recover Naver-Stokes Equation through Chapman Enskog expansion.

$$\begin{aligned}
&\delta N_\alpha(\vec{q},t) = w_i\left(\frac{c_\alpha^i F^i}{c_s^2} + \frac{c_\alpha^i c_\alpha^j - c_s^2\delta^{ij}}{2c_s^4}\right)\\
&\sum_{\alpha=1}^{q} f^{eq}(\vec{q},t) = \rho\\
&\sum_{\alpha=1}^{q} f^{eq}(\vec{q},t)c_\alpha^i = \rho u^i\\
&\sum_{\alpha=1}^{q} f^{eq}(\vec{q},t)c_\alpha^i c_\alpha^j = \rho c_s^2 g^{ij} + \rho(u^i + \frac{1}{2}\frac{F^i}{\rho})(u^j + \frac{1}{2}\frac{F^j}{\rho})
\end{aligned} \tag{2.17}$$