

# 4. Volumetric Lattice Boltzmann Models in General Curvature

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February 2, 2026

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# 1 Gauss-Hermite quadrature rule

This section would show the process the 1 dimension n orders Gauss-Hermite quadrature to 3 dimension n orders Gauss-Hermite quadrature rule. Below the equation is the basic quadrature rule for solving integration.

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

Above is the one dimension n orders Gauss-Hermite quadrature rule, where the function  $P^{2n-1}$  is any  $2n-1$  order polynomials, so the rule is used for any  $2n-1$  orders polynomials. And 1 dimension n orders Gauss-Hermite quadrature rule can be promoted to any function which order is smaller than  $2n-1$ . List below will show some unknown information 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 $H^{(n)}(r)$
Weights	$w_i$	$\frac{n!}{(nH^{(n-1)}(r))^2}$

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

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

The variables  $r_i$  is the roots of 1 dimension n orders Hermite polynomial. A thing you have to realize is n orders Hermite polynomial have n roots i.e. the order of n order Hermite polynomial is equal to number of roots.

**3 dimensions n orders Hermite polynomials** The definition of 3 dimensions n orders Hermite polynomials is described as below :

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

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

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

For any  $2n - 1$  order polynomial, 1 dimension n order Gauss-Hermite quadrature rule can solve integration which integration domain from  $-\infty$  to  $\infty$ .

**Gauss-Hermite promoted to high dimensions** Assume a volume integration for hole 3 dimensions space :

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

Bacause the summiton have a limit number terms, so the integration can be putted into summition. we have

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

Now we have to use the property of exponential function :

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

Using 1 dimension n orders Gauss-Hermite quadrature rule to each integration pointed to different direction. We have

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

where  $(2n_a - 1) > a$ ,  $(2n_b - 1) > b$ ,  $(2n_c - 1) > c$ . The detail as below:

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

where  $x_i$  is the root of 1 dimension  $n_a$  order Hermite function. Usually, for each 1 dimension Gauss-Hermite quadrature rule, we take the order as the order of integrated function i.e., take the max order among the polynomial terms, so we can take the summition to deal with the inrtegration above :

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

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

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \omega(x, y) x^2 y = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \frac{1}{\sqrt{2\pi}} e^{-\frac{(x^2+y^2)}{2}} x^2 y = (w_1 y_1 + w_2 y_2) (w_1 x_1^2 + w_2 x_2^2)$$

## 2 Momentum Loss of Distribution Function in Propagation

In general curvilinear coordinates, for macroscopic values i.e.,  $\rho, \rho \vec{u}$  exist the loss due to the curvature and uniform properties. And this paper shows the value below:

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

where q is the non-dimension position, and the origin form of it is  $\vec{q} = (q_1, q_2, q_3)$ . The value  $N^*$  represents post-collision distribution function. We can review the Lattice Boltzman Equation-BGK

(LBGK) and see the position of the value in the equation.

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

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

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

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

### Definition 2.1.

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

we call the value is "non-dimension change of curvature tangent vector", where  $\vec{g}^j$  can be defined as below:

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

Substitute the vector in equation (2.4)

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

### Definition 2.2.

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

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

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

The pre-streaming distribution function is different from the post-collision function, but the sum of distribution along the discrete velocity space is same for two function set. we can realize the fact that desity can't loss in streaming step at cuvelinear coordinate. But this paper defines two values about inner and outer momentum loss at the point  $(q, t)$  as shown, prepared for proving inertial force.

**Definition 2.3.**

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

where, for the discrete particle velocity set

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

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

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

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

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

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, impose two "symbols" for inner and outer momentum loss; then define the form of velocity space-discretized force field , and proved the inertial force using the mometum loss finally. 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

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

where  $\hat{g}_i = \frac{\vec{g}_i}{|\vec{g}_i|}$  is the unit vector in the  $i$ -th coordinate direction. This form uses a time difference (division by  $\Delta t$ ) 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.** prove of the equation

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

The principle of the derivation can apart into three things :

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

$$\begin{aligned}
\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) (\vec{e}_\alpha(\vec{q}) - \vec{e}_\alpha(\vec{q} - \vec{e}_\alpha \delta t)) + \sum_{\alpha=1}^q N_\alpha^\star(\vec{q}, t) (\vec{e}_\alpha(\vec{q} + \vec{e}_\alpha \delta t) - \vec{e}_\alpha(\vec{q})) \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) (\vec{e}_\alpha(\vec{q}) - \vec{e}_\alpha(\vec{q} - \vec{e}_\alpha \delta t)) + \sum_{\alpha=1}^q N_\alpha^\star(\vec{q}, t) (\vec{e}_\alpha(\vec{q} + \vec{e}_\alpha \delta t) - \vec{e}_\alpha(\vec{q})) \right) \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}) \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) \right. \\
&\quad \left. + \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) \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{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) \\
&= \frac{-1}{2} \left( \sum_{\alpha=1}^q N_\alpha(\vec{q}, t) (c_\alpha^i \Theta_i^j(\vec{q} - \vec{e}_\alpha \delta t, \vec{q})) + \sum_{\alpha=1}^q N_\alpha^\star(\vec{q}, t) (c_\alpha^i \Theta_i^j(\vec{q} + \vec{e}_\alpha \delta t, \vec{q})) \right)
\end{aligned} \tag{2.15}$$

## 2.1 Basic Equation for Curvilinear Coordinate

$$\begin{aligned}
\delta N_\alpha(\vec{q}, t) &= w_i \left( \frac{c_\alpha^i F^i}{c_s^2} + \frac{c_\alpha^i c_\alpha^j - c_s^2 \delta^{ij}}{2c_s^4} \right) \\
\sum_{\alpha=1}^q f^{eq}(\vec{q}, t) &= \rho \\
\sum_{\alpha=1}^q f^{eq}(\vec{q}, t) c_\alpha^i &= \rho u^i \\
\sum_{\alpha=1}^q f^{eq}(\vec{q}, t) c_\alpha^i c_\alpha^j &= \rho c_s^2 g^{ij} + \rho(u^i + \frac{1}{2} \frac{F^i}{\rho})(u^j + \frac{1}{2} \frac{F^j}{\rho})
\end{aligned} \tag{2.16}$$