Volumetric Lattice Boltzmann Models in General Curvilinear Coordinates: Theoretical Formulation

Hudong Chen

Dassault Systemes, Waltham, MA, United States

Front. Appl. Math. Stat. 7:691582 doi: 10.3389/fams.2021.691582
Published: 16 June 2021

A volumetric formulation for lattice Boltzmann models on general curvilinear coordinates is presented, preserving one-to-one advection and recovering the Navier–Stokes equations in the hydrodynamic limit.

Presenter: Chen Peng Chung

Outline

Introduction & Motivation

Core Problem

For standard Lattice Boltzmann Methd, Because the velocity direction set, it only was used in Cartesian coordinates.However, this paper show the basic theoretical formulation to extend the limitation. In **general curvilinear coordinates**, we have to consider:

- Curvature effects
- Nonuniform grid properties

Key Question

How to maintain **momentum conservation** in the streaming step of LBM when using curvilinear coordinates?

Solution Approach

Define a **velocity-space discretized force field** to compensate for the momentum loss (interpreted as an **inertial force**), and make it be tangent with curve line.

Lattice Boltzmann BGK Equation

The standard LBGK equation in curvilinear coordinates:

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

where the correction term is defined as:

$$\delta N_\alpha(\vec{q}, t) \equiv N_\alpha(\vec{q}, t) - N^\star_\alpha(\vec{q} - \vec{e}_\alpha \delta t, t-1)$$

- $\vec{q}$: nondimensional position (q_1, q_2, q_3)
- $N^\star$: **post-collision** distribution function
- Ω_α : collision operator
- $\vec{e}_\alpha$: discrete velocity directions in curvilinear coordinate.

where $\delta N(\vec{q}, t)$ is the source of momentum loss.

Mass Conservation vs Momentum Loss

Mass Conservation (✓)

$$\sum_{\alpha=0}^{q-1} \delta N_\alpha(\vec{q}, t) = 0$$

Reason: Sum of distributions over velocity space is conserved.

Momentum Loss (×)

$$\sum_{\alpha=1}^{q} \vec{e}_\alpha \, \delta N_\alpha \neq 0$$

Reason: Discrete velocity vectors $\vec{e}_\alpha$ vary (in direction and magnititude)with position in curvilinear coords!

Key Insight: $N_\alpha(\vec{q}, t) \;\neq\; N^\star_\alpha(\vec{q} - \vec{e}_\alpha \delta t, t - 1)$

Pre-streaming $\neq$ Post-collision at different positions

Due to curvilinearity, though the amount of particles advected from cell $\vec{q}$ is exactly equal to what is arrived at cell $\vec{q} + \vec{e}_\alpha$, the momentum is in fact changed along the way

Definition: Nondimensional Curvature Change

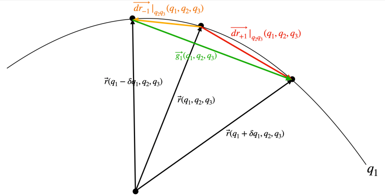
Definition

The **nondimensional change of curvature tangent vector**:

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

where the **co-tangent basis vector** $\vec{g}^j$ is:

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



$$\vec{g}_i = \frac{\overrightarrow{dr_{+1}} - \overrightarrow{dr_{-1}}}{|\overrightarrow{dr_{+1}} - \overrightarrow{dr_{-1}}|} \cdot \frac{|\overrightarrow{dr_{+1}}| + |\overrightarrow{dr_{-1}}|}{2 \cdot \Delta l} \quad \begin{array}{ll} > 1 & \text{: curvilinear rate exist !} \\ = 0 & \text{: curvilinear rate} = 0 \end{array}$$

$$\vec{e}_i \equiv \frac{\vec{g}_i}{|\vec{g}_i|}$$

- $\vec{g}_i$: curvatue tangent basis vector (tangent to coordinate curves)
- $\vec{g}^j$: co-tangent basis vector (normal to coordinate surfaces)
- Θ_i^j measures how the tangent vector changes along $\vec{e}_\alpha$

Definition: Momentum Loss

Definition

Total Momentum Loss at point $(\vec{q}, t)$:

$$\vec{M}_{\text{Loss}}(\vec{q}, t) \equiv \sum_{\alpha=1}^{q} \left[N_\alpha(\vec{q}, t)\, \vec{e}_\alpha(\vec{q}) - N^\star_\alpha(\vec{q} - \vec{e}_\alpha \delta t, t-1)\, \vec{e}_\alpha(\vec{q} - \vec{e}_\alpha \delta t)\right]$$

- Momentum carried by particles **arriving** at $\vec{q}$
- Minus momentum carried by particles **leaving** from $\vec{q} - \vec{e}_\alpha \delta t$
- Difference arises because $\vec{e}_\alpha(\vec{q}) \neq \vec{e}_\alpha(\vec{q} - \vec{e}_\alpha \delta t)$

For inducing the inertial force, the author adopt the definition as below :

Definition

$$\vec{M}_{\text{Loss}}(\vec{q}, t) \equiv \sum_{\alpha=1}^{q} \vec{e}_\alpha(\vec{q}, t) \delta N_\alpha(\vec{q}, t)$$

Inner & Outer Momentum Loss

The paper separates momentum loss into **two contributions**:

Definition

Inner Momentum Loss (particles entering):

$$\mathcal{J}(\vec{q})\, \vec{\chi}^{\text{in}}(\vec{q}, t) \equiv -\sum_{\alpha=1}^{q} N_\alpha(\vec{q}, t) \cdot \left(\vec{e}_\alpha(\vec{q}) - \vec{e}_\alpha(\vec{q} - \vec{e}_\alpha \delta t)\right)$$

Definition

Outer Momentum Loss (particles leaving):

$$\mathcal{J}(\vec{q})\, \vec{\chi}^{\text{out}}(\vec{q}, t) \equiv -\sum_{\alpha=1}^{q} \left(\vec{e}_\alpha(\vec{q} + \vec{e}_\alpha \delta t) - \vec{e}_\alpha(\vec{q})\right) \cdot N^\star_\alpha(\vec{q}, t)$$

where $\mathcal{J}$ is the Volume element in gerneral coordinate.

Discrete Velocity in Curvilinear Coordinates

The **discrete particle velocity set** in curvilinear coordinates:

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

- c_α^i : lattice velocity components (integers like $0, \pm 1$)
- $\vec{g}_i$: local covariant basis vectors
- $\Delta x / \Delta t$: lattice speed ratio

Important

Unlike Cartesian coordinates, $\vec{e}_\alpha$ depends on position $\vec{q}$ through the basis vectors $\vec{g}_i(\vec{q})$.

The author imposes the **momentum constraint** for the streaming step:

$$\sum_{\alpha=1}^{q} \vec{e}_\alpha(\vec{q})\,\delta N_\alpha(\vec{q}) = \mathcal{J} \cdot \frac{\vec{\chi}^{\text{in}}(\vec{q},t) + \vec{\chi}^{\text{out}}(\vec{q},t)}{2}$$

Expanding:

$$= \mathcal{J} \cdot \frac{{\color{blue}-\sum_\alpha N_\alpha(\vec{q})\,(\vec{e}_\alpha(\vec{q}) - \vec{e}_\alpha(\vec{q} - \vec{e}_\alpha\delta t))}{\color{red}-\sum_\alpha N^\star_\alpha(\vec{q})\,(\vec{e}_\alpha(\vec{q} + \vec{e}_\alpha\delta t) - \vec{e}_\alpha(\vec{q}))}}{2}$$

- Blue: contribution from pre-collision distribution
- Red: contribution from post-collision distribution

Inertial Force Definition

Definition

The **inertial force** produced by curvature in curvilinear coordinates:

$$\boxed{F^i(\vec{q},t) \equiv \sum_{\alpha=1}^{q} \vec{e}_\alpha \delta N_\alpha(\vec{q},t) = \frac{\vec{\chi}^{\text{in}}(\vec{q},t) + \vec{\chi}^{\text{out}}(\vec{q},t)}{2} \cdot \vec{g}^{\,i}(\vec{q})}$$

Physical Interpretation:

- This force represents the **inertial force** arising from curvilinear coordinates
- the reason why this term exist is difference between pre-streaming and post-collision distributojn function.
- Compensates for the "loss" in momentum during streaming

My problem about definiton of force

$$\mathcal{J}(\vec{q})F^i(\vec{q},t) \equiv \frac{\text{Momentum Loss}}{\Delta t} \cdot \vec{e}_j$$

Final Force Formula

After derivation, the force field becomes:

$$\boxed{\mathcal{J}(\vec{q})F^j(\vec{q},t) = \frac{-1}{2}\left(\sum_\alpha N_\alpha\, c^i_\alpha \Theta^j_i(\vec{q}-\vec{e}_\alpha\delta t,\vec{q}) + \sum_\alpha N^\star_\alpha\, c^i_\alpha \Theta^j_i(\vec{q}+\vec{e}_\alpha\delta t,\vec{q})\right)}$$

Key Components:

Symbol	Meaning
$\mathcal{J}$	volume of the cell centered at $\vec{x}(\vec{q})$,
c^i_α	Lattice velocity component
Θ^j_i	change of Curvature change tensor
N_α	Post-streaming distribution
$N^\star_\alpha$	Post-collision(pre-streaming) distribution

Solving the addition term δN_α

To recover the full viscous Navier-Stokes equation, an additional constraint on the **momentum flux** is needed:

Momentum flux constraint (Eq.29):

$$\sum_\alpha c^i_\alpha c^j_\alpha \delta N_\alpha(\vec{q},t) = \mathcal{J}(\vec{q})\left[\delta\Pi^{ij}(\vec{q},t) + \delta\Pi^{ji}(\vec{q},t)\right]$$

Non-equilibrium stress tensor (Eq.30):

$$\delta\Pi^{ij}(\vec{q},t) = -\frac{1}{2}\left(1 - \frac{1}{2\tau}\right)\sum_\alpha c^i_\alpha c^k_\alpha \left[\Theta^j_k(\vec{q}+\vec{e}_\alpha\delta t,\vec{q}) - \Theta^j_k(\vec{q}-\vec{e}_\alpha\delta t,\vec{q})\right] f^{\text{eq}}_\alpha(\vec{q},t)$$

Specific form of δN_α (Eq.31):

$$\boxed{\delta N_\alpha(\vec{q},t) = w_\alpha \mathcal{J}(\vec{q})\left[\frac{c^i_\alpha F^i(\vec{q},t)}{T_0} + \left(\frac{c^i_\alpha c^k_\alpha}{T_0} - \delta^{ik}\right)\frac{\delta\Pi^{ik}(\vec{q},t)}{T_0}\right]}$$

This form satisfies the moment constraints of (13), (13)

Equilibrium Distribution & Moment Constraints

Fundamental moment conditions (to recover Euler & Navier-Stokes):

$$\sum_{\alpha} f_{\alpha} = \rho$$

$$\sum_{\alpha} \vec{e}_{\alpha} f_{\alpha} = \rho \vec{u}(\vec{q}, t) \Rightarrow \sum_{\alpha} c^{i}_{\alpha} f_{\alpha} = \rho U^{i}$$

$$\sum_{\alpha} c^{i}_{\alpha} c^{j}_{\alpha} f^{\text{eq}}_{\alpha} = \Pi^{ij,\text{eq}} = g^{ij} \rho T_0 + \rho \tilde{U}^{i} \tilde{U}^{j}$$

where the **shifted velocity**: $\tilde{U}^{i}(\vec{q}, t) = U^{i}(\vec{q}, t) + \frac{1}{2} a^{i}(\vec{q}, t), \quad \text{with } \rho a^{i} \equiv F^{i}$

Equilibrium distribution form:

$$\boxed{f^{\text{eq}}_{\alpha} = \rho w_{\alpha} \left[1 + \frac{c^{i}_{\alpha} U^{i}}{T_0} + \frac{1}{2T_0} \left(\frac{c^{i}_{\alpha} c^{j}_{\alpha}}{T_0} - \delta^{ij} \right) \left[(g^{ij} - \delta^{ij}) T_0 + \tilde{U}^{i} \tilde{U}^{j} \right] \right]}$$

This form satisfies all the fundamental moment conditions above.

Fundamental moment conditions (to recover Euler & Navier-Stokes):

$$\sum_\alpha f_\alpha(\vec{r}, t) = \rho$$

$$\sum_\alpha c^i_\alpha f_\alpha = \rho U^i$$

$$\sum_\alpha c^i_\alpha c^j_\alpha f^{\mathrm{eq}}_\alpha = \rho \left(U^i U^j + c_s^2 \delta_{ij} \right)$$

Equilibrium distribution form:

$$\boxed{f^{\mathrm{eq}}_\alpha = \rho w_\alpha \left[1 + \frac{c^i_\alpha U^i}{c_x^2} + \frac{(U^i U^j + (\theta - 1)\delta_{ij})(c^i_\alpha c^j_\alpha - c_s^2 \delta_{ij})}{2 c_s^4} \right]}$$

This form satisfies all the fundamental moment conditions above.

Summary & Key Takeaways

Main Contributions

1. Identified **momentum loss** in streaming step for curvilinear LBM
2. Introduced **curvature change tensor** Θ^j_i to quantify geometric effects
3. Derived **velocity-space discretized force field** to restore conservation

Physical Insight

The force field F^i acts as an **inertial force** (like centrifugal force), arising purely from the curvilinear coordinate system.

Practical Use

Add correction term δN_α to LBGK equation:

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

Appendix: Derivation of Force Field Equation

Target Equation:

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

Derivation Principles:

1. $\sum_{\alpha=1}^{q} \vec{e}_\alpha(\vec{q})\,\delta N_\alpha(\vec{q},t) \equiv \text{Momentum Loss of the Streaming Step}$
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: $\mathcal{J}(\vec{q})F^{i} \equiv \frac{\text{Momentum Loss}}{\Delta t}\cdot\vec{e}_j\frac{1}{|\vec{g}_j|}$

Step-by-step derivation:

$$\mathcal{J}(\vec{q})F^1 = \sum_{\alpha=1}^{q} \vec{e}_\alpha(\vec{q})\delta N_\alpha(\vec{q},t) \cdot \vec{g}^{\,1} = \sum_{\alpha=1}^{q} \vec{e}_\alpha(\vec{q})\delta N_\alpha(\vec{q},t) \cdot \frac{\vec{g_2} \times \vec{g_3}}{(\vec{g_2} \times \vec{g_3}) \cdot \vec{g}_1}$$

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

$$\cdot \frac{\vec{g_2} \times \vec{g_3}}{(\vec{g_2} \times \vec{g_3}) \cdot \vec{g}_1}$$

Continuing:

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

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

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

Using Θ_i^j definition:

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

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

Final Result:

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