

## Lecture 3: Generalized Lattice Boltzmann Equation

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# Motivation

- To overcome the shortcomings of the BGK model;
- To improve numerical stability;
- To gain maximum freedom of the model;
- To present a systematic analysis of the LBE method.

# Dissipation, Dispersion, and Galilean Invariance

- Dissipation: Hyperviscosity

$$\nu(\mathbf{k}) = \nu_0 - \nu_1 k^2 + \nu_2 k^4 + \dots + (-1)^n \nu_n k^{2n} + \dots$$

- Galilean Invariance: In reference frame with velocity  $V$

$$\begin{aligned} \exp[i(\mathbf{k} \cdot \mathbf{r} - \omega t)] &\implies \exp[i(\mathbf{k} \cdot \mathbf{r} - \omega t) - i\mathbf{g}(\mathbf{k})\mathbf{k} \cdot \mathbf{V}t] \\ g(\mathbf{k}) &= g_0 - g_1 k^2 + g_2 k^4 + \dots + (-1)^n g_n k^{2n} + \dots \end{aligned}$$

- **Isotropy:** Dependence of transport coefficients  $[\nu(\mathbf{k}), \eta(\mathbf{k}), c_s(\mathbf{k}), \text{ and } g(\mathbf{k})]$  on the direction of  $\mathbf{k}$
- **Analysis:** **Linear Dispersion Equation & Generalized Hydrodynamics**<sup>1,2,3,4,5,6</sup>

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<sup>1</sup>L.-S. Luo, H. Chen, S. Chen, G. Doolen, and Y.-C. Lee, *Phys. Rev. A* **43**:7097 (1991).

<sup>2</sup>P. Grosfilis and P. Lallemand, *Europhys. Lett.* **24**:473 (1993).

<sup>3</sup>S.P. Das, H.J. Bussemaker, and M.H. Ernst, *Phys. Rev. E* **48**:245 (1993).

<sup>4</sup>P. Grosfilis, J.P. Boon, R. Brito, and M.H. Ernst, *Phys. Rev. E* **48**:2655 (1993).

<sup>5</sup>P. Behrend, R. Harris, and P.B. Warren, *Phys. Rev. E* **50**:4586 (1994).

<sup>6</sup>L.-S. Luo and P. Lallemand, *Phys. Rev. E* **61**:6546 (2000).

# Lattice Boltzmann Equation

Lattice Boltzmann Equation in particle velocity space:

$$f_{\alpha}(\mathbf{x}_i + \mathbf{e}_{\alpha}, t + 1) = f_{\alpha}(\mathbf{x}_i, t) + \Omega_{\alpha}(f) \quad (1)$$

$$\rho(\mathbf{x}_i, t) = \sum_{\alpha} f_{\alpha}(\mathbf{x}_i, t)$$

$$\rho \mathbf{u}(\mathbf{x}_i, t) = \sum_{\alpha} \mathbf{e}_{\alpha} f_{\alpha}(\mathbf{x}_i, t)$$

$$|f(\mathbf{x}_i + \mathbf{e}_{\alpha}, t + 1)\rangle = |f(\mathbf{x}_i, t)\rangle + |\Omega(f)\rangle \quad (2)$$

## Moment Space

Mapping from the **distribution functions**  $\{f_\alpha | \alpha = 1, 2, \dots, b\}$  to **moments**  $\{\varrho_\alpha | \alpha = 1, 2, \dots, b\}$  (for 9-velocity model):

$$\begin{aligned}
 \mathbf{M} &\equiv \begin{pmatrix} \langle \rho | \\ \langle e | \\ \langle \varepsilon | \\ \langle j_x | \\ \langle j_y | \\ \langle q_y | \\ \langle p_{xx} | \\ \langle p_{xy} | \end{pmatrix} \equiv \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -4 & -1 & -1 & -1 & -1 & 2 & 2 & 2 & 2 \\ 4 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \\ 0 & 0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 \\ 0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \end{pmatrix} \\
 &\equiv (|\rho\rangle, |e\rangle, |\varepsilon\rangle, |j_x\rangle, |j_y\rangle, |q_y\rangle, |p_{xx}\rangle, |p_{xy}\rangle)^T \\
 | \varrho \rangle &= \mathbf{M} | f \rangle \quad | f \rangle = \mathbf{M}^{-1} | \varrho \rangle
 \end{aligned}$$

# Moments

The moments in the 9-velocity model:

Order	Quantity	
0	<b>Density:</b>	$\rho = \langle \rho   f \rangle = \langle f   \rho \rangle$
2	Energy:	$e = \langle e   f \rangle = \langle f   e \rangle$
4	Energy Square:	$\varepsilon = \langle \varepsilon   f \rangle = \langle f   \varepsilon \rangle$
1	<b><i>x</i>-Momentum:</b>	$j_x = \langle j_x   f \rangle = \langle f   j_x \rangle$
3	<i>x</i> -Heat Flux:	$q_x = \langle q_x   f \rangle = \langle f   q_x \rangle$
1	<b><i>y</i>-Momentum:</b>	$j_y = \langle j_y   f \rangle = \langle f   j_y \rangle$
3	<i>y</i> -Heat Flux:	$q_y = \langle q_y   f \rangle = \langle f   q_y \rangle$
2	Stress:	$p_{xx} = \langle p_{xx}   f \rangle = \langle f   p_{xx} \rangle$
2	Stress:	$p_{xy} = \langle p_{xy}   f \rangle = \langle f   p_{xy} \rangle$

# Generalized BGK Approximation in Moment Space

Relaxation process of moments:

$$\begin{pmatrix} \Delta \rho \\ \Delta e \\ \Delta \varepsilon \\ \Delta j_x \\ \Delta q_x \\ \Delta j_y \\ \Delta q_y \\ \Delta p_{xx} \\ \Delta p_{xy} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -s_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -s_3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -s_5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -s_7 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -s_8 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -s_9 \end{pmatrix} \begin{pmatrix} \delta \rho \\ \delta e \\ \delta \varepsilon \\ \delta j_x \\ \delta q_x \\ \delta j_y \\ \delta q_y \\ \delta p_{xx} \\ \delta p_{xy} \end{pmatrix}$$

$$|\delta \varrho\rangle \equiv |\varrho\rangle - |\varrho^{(eq)}\rangle$$

$$|\Delta \varrho\rangle = \mathbf{S} [|\varrho\rangle - |\varrho^{(eq)}\rangle]$$

<sup>7</sup> D. d'Humières, in *Rarefied Gas Dynamics: Theory and Simulations*, Prog. Astronaut. Aeronaut. Vol. **159**, edited by B.D. Shizgal and D.P. Weaver (AIAA, Washington, D.C. 1992).

<sup>8</sup> L.-S. Luo and P. Lallemand, *Phys. Rev. E* **61**:6546 (2000).

Luo, NIA: LBE Method for CFD, CAB-TUB, Aug. 7-12, 2003

## Equilibriums in Moment Space

The equilibrium functions depend only upon conserved moments:

$$\begin{aligned}e^{(\text{eq})} &= \frac{1}{\langle e|e \rangle} [\alpha_2 \langle \rho|\rho \rangle \rho + \gamma_2 (\langle j_x|j_x \rangle j_x^2 + \langle j_y|j_y \rangle j_y^2)] = \frac{1}{4} \alpha_2 \rho + \frac{1}{6} \gamma_2 (j_x^2 + j_y^2) \\ \varepsilon^{(\text{eq})} &= \frac{1}{\langle \varepsilon|\varepsilon \rangle} [\alpha_3 \langle \rho|\rho \rangle \rho + \gamma_4 (\langle j_x|j_x \rangle j_x^2 + \langle j_y|j_y \rangle j_y^2)] = \frac{1}{4} \alpha_3 \rho + \frac{1}{6} \gamma_4 (j_x^2 + j_y^2) \\ q_x^{(\text{eq})} &= \frac{\langle j_x|j_x \rangle}{\langle q_x|q_x \rangle} c_1 j_x = \frac{1}{2} c_1 j_x \\ q_y^{(\text{eq})} &= \frac{\langle j_y|j_y \rangle}{\langle q_y|q_y \rangle} c_1 j_y = \frac{1}{2} c_1 j_y \\ p_{xx}^{(\text{eq})} &= \frac{1}{\langle p_{xx}|p_{xx} \rangle} (\langle j_x|j_x \rangle j_x^2 - \langle j_y|j_y \rangle j_y^2) = \frac{3}{2} \gamma_1 (j_x^2 - j_y^2) \\ p_{xy}^{(\text{eq})} &= \frac{\gamma_3 \sqrt{\langle j_x|j_x \rangle \langle j_y|j_y \rangle}}{\langle p_{xx}|p_{xx} \rangle} (j_x j_y) = \frac{3}{2} \gamma_3 (j_x j_y)\end{aligned}$$

There are 7 adjustable parameters in the model:  $\alpha_2$ ,  $\alpha_3$ ,  $c_1$ ,  $\gamma_1$ ,  $\gamma_2$ ,  $\gamma_3$ ,  $\gamma_4$ .

## Generalized Lattice Boltzmann Equation

Generalized Lattice Boltzmann Equation with multiple relaxation parameters:

$$|f(\mathbf{x}_i + \mathbf{e}_\alpha, t + 1)\rangle = |f(\mathbf{x}_i, t)\rangle + M^{-1}S [| \varrho(\mathbf{x}_i, t)\rangle - | \varrho^{(\text{eq})}(\mathbf{x}_i, t)\rangle] \quad (3)$$

- Initialize  $|f\rangle$ ;
- Project  $|f\rangle$  to moments by  $| \varrho\rangle = M|f\rangle$  and compute the equilibrium  $| \varrho^{(\text{eq})}\rangle$ ;
- Collision in moment space (multiple-parameter relaxation)

$$| \Delta \varrho\rangle \equiv S [| \varrho\rangle - | \varrho^{(\text{eq})}\rangle]$$

- Streaming in velocity space:

$$|f(\mathbf{x}_i + \mathbf{e}_\alpha, t + 1)\rangle = |f(\mathbf{x}_i, t)\rangle + M^{-1}| \Delta \varrho\rangle$$

## Linearized Lattice Boltzmann Equation

Suppose the system in uniform state  $\rho$  and  $V = (V_x, V_y)$ , and

$$|f\rangle = |f^{(0)}\rangle + |\delta f\rangle$$

$$|\delta f(\mathbf{r}_j + \mathbf{e}_\alpha, t + 1)\rangle = |\delta f(\mathbf{r}_j, t)\rangle + M^{-1}CM|\delta f(\mathbf{r}_j, t)\rangle$$

In Fourier space:

$$A|\delta f(\mathbf{k}, t + 1)\rangle = |\delta f(\mathbf{k}, t)\rangle + M^{-1}CM|\delta f(\mathbf{k}, t)\rangle$$

$$C_{\alpha\beta} = \frac{\langle \varrho_\alpha | \varrho_\alpha \rangle}{\langle \varrho_\beta | \varrho_\beta \rangle} \frac{\partial}{\partial \varrho_\alpha} [\varrho_\beta - \varrho_\beta^{(\text{eq})}] \quad A_{\alpha\beta} = \exp(i\mathbf{e}_\alpha \cdot \mathbf{k}) \delta_{\alpha\beta}$$

The Linearized Lattice Boltzmann Equation:

$$|\delta f(\mathbf{k}, t + 1)\rangle = L|\delta f(\mathbf{k}, t)\rangle \quad L = A^{-1}[I + M^{-1}CM] \quad (4)$$

## Eigenvalue Problem of Linearized LBE

The eigenvalue problem of the linearized evolution operator:

$$\det[\mathbf{L} - z\mathbf{I}] = 0$$

Hydrodynamic modes ( $z_\alpha = 1$ ) of  $\mathbf{L}$  at  $\mathbf{k} = (k \cos \theta, k \sin \theta) \rightarrow \mathbf{0}$ :

$$|\varrho_T\rangle = \cos \theta |j_x\rangle - \sin \theta |j_y\rangle \equiv |j_T\rangle$$

$$|\varrho_\pm\rangle = |\rho\rangle \pm (\cos \theta |j_x\rangle + \sin \theta |j_y\rangle) \equiv |\rho\rangle \pm |j_L\rangle$$

$$|\varrho_T(t)\rangle = z_T^t |\varrho_T(0)\rangle = \exp[-ik(gV \cos \phi)t] \exp(-\nu k^2 t) |\varrho_T(0)\rangle$$

$$|\varrho_\pm(t)\rangle = z_\pm^t |\varrho_\pm(0)\rangle = \exp[\pm ik(c_s \pm gV \cos \phi)t] \exp[-(\nu/2 + \zeta)k^2 t] |\varrho_\pm(0)\rangle$$

Transport coefficients  $\nu$ ,  $\zeta$ ,  $c_s$ , and  $g$  are functions of wavevector  $\mathbf{k}$ .

## Determining Adjustable Parameters

Galilean invariance of the phases in the transverse mode ( $z_T$ ) and the sound modes ( $z_{\pm}$ ) up to  $k$  leads to:

$$\gamma_1 = \gamma_3 = \frac{2}{3}$$

$$\gamma_2 = 18$$

Isotropy of the attenuation of the transverse mode ( $z_T$ ) and Galilean invariance of the attenuation of the sound modes ( $z_{\pm}$ ) lead to

$$c_1 = -2 \quad (c_s = 1/\sqrt{3})$$

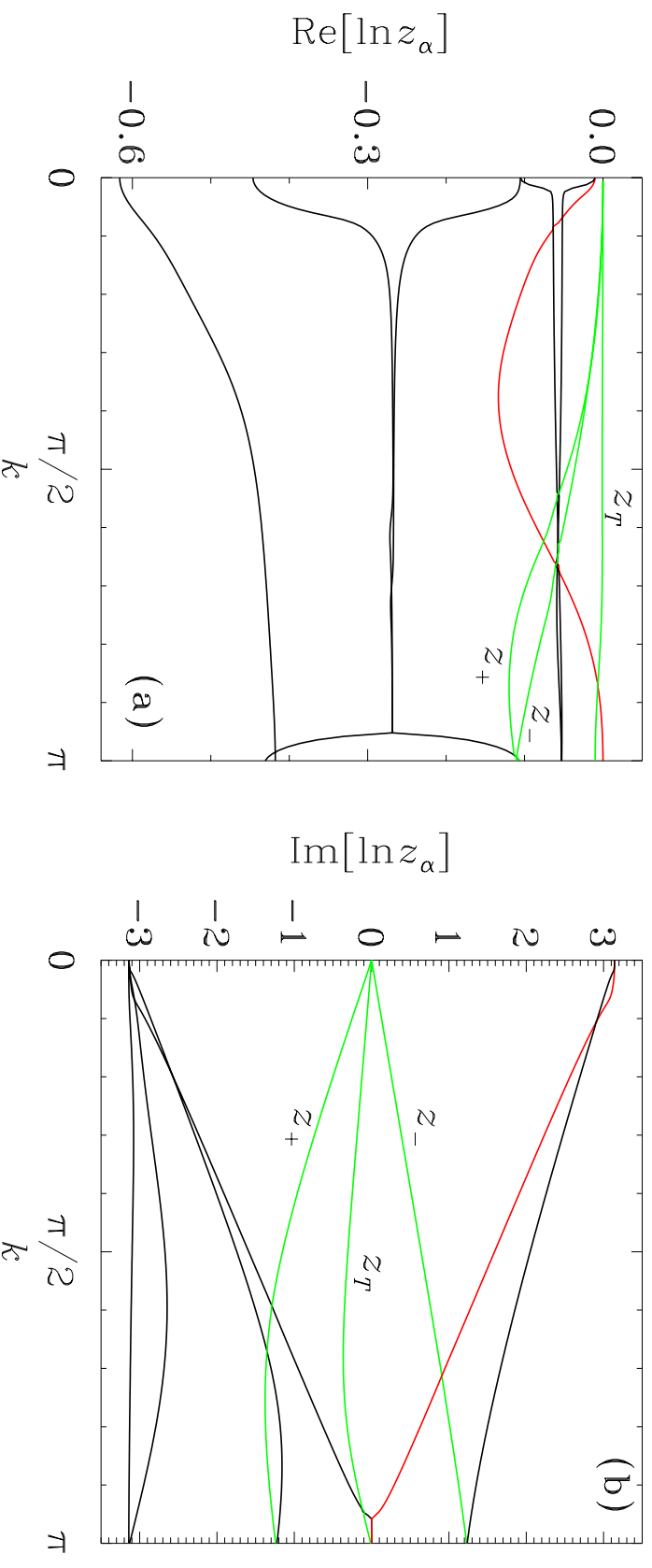
$$\alpha_2 = -8$$

Remaining adjustable parameters:  $\alpha_3$  and  $\gamma_4$  (in  $\epsilon^{(\text{eq})}$ ). If

$$\alpha_3 = 4 \quad \gamma_4 = -18 \quad s_{\alpha} = \frac{1}{\tau}$$

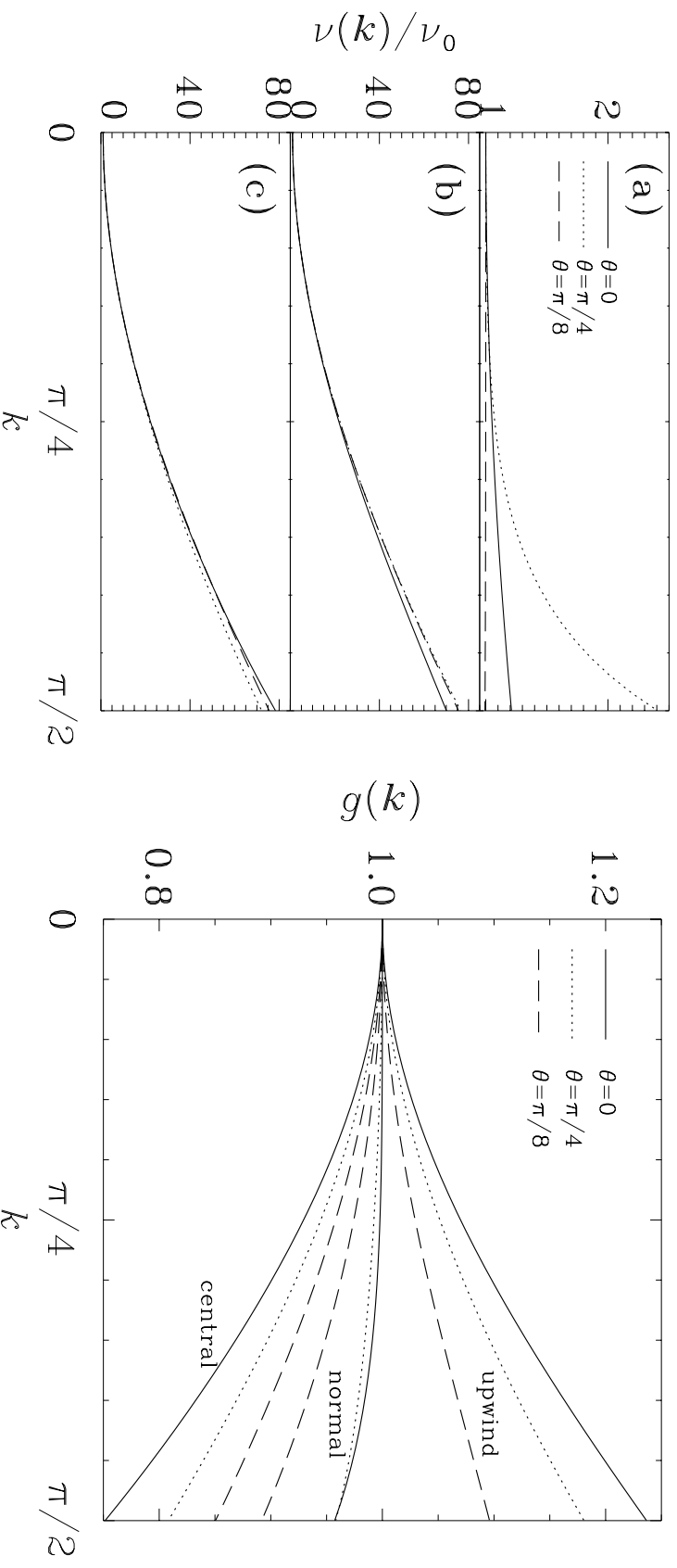
Generalized lattice Boltzmann equation degenerates to a lattice BGK model.

## Behaviors of Eigenvalues of $L$



Logarithmic eigenvalues of the nine-velocity model. The values of the parameters are  $\alpha_2 = -8$ ,  $\alpha_3 = 4$ ,  $c_1 = -2$ ,  $\gamma_1 = \gamma_3 = 2/3$ ,  $\gamma_2 = 18$ , and  $\gamma_4 = -18$ . The relaxation parameters are:  $s_2 = 1.64$ ,  $s_3 = 1.54$ ,  $s_5 = s_7 = 1.9$ , and  $s_8 = s_9 = 1.99$ . The streaming velocity  $V$  is parallel to  $k$  with  $V = 0.2$ , and  $k$  is along the  $x$  axis. (a)  $\text{Re}(\ln z_\alpha)$  and (b)  $\text{Im}(\ln z_\alpha)$ .

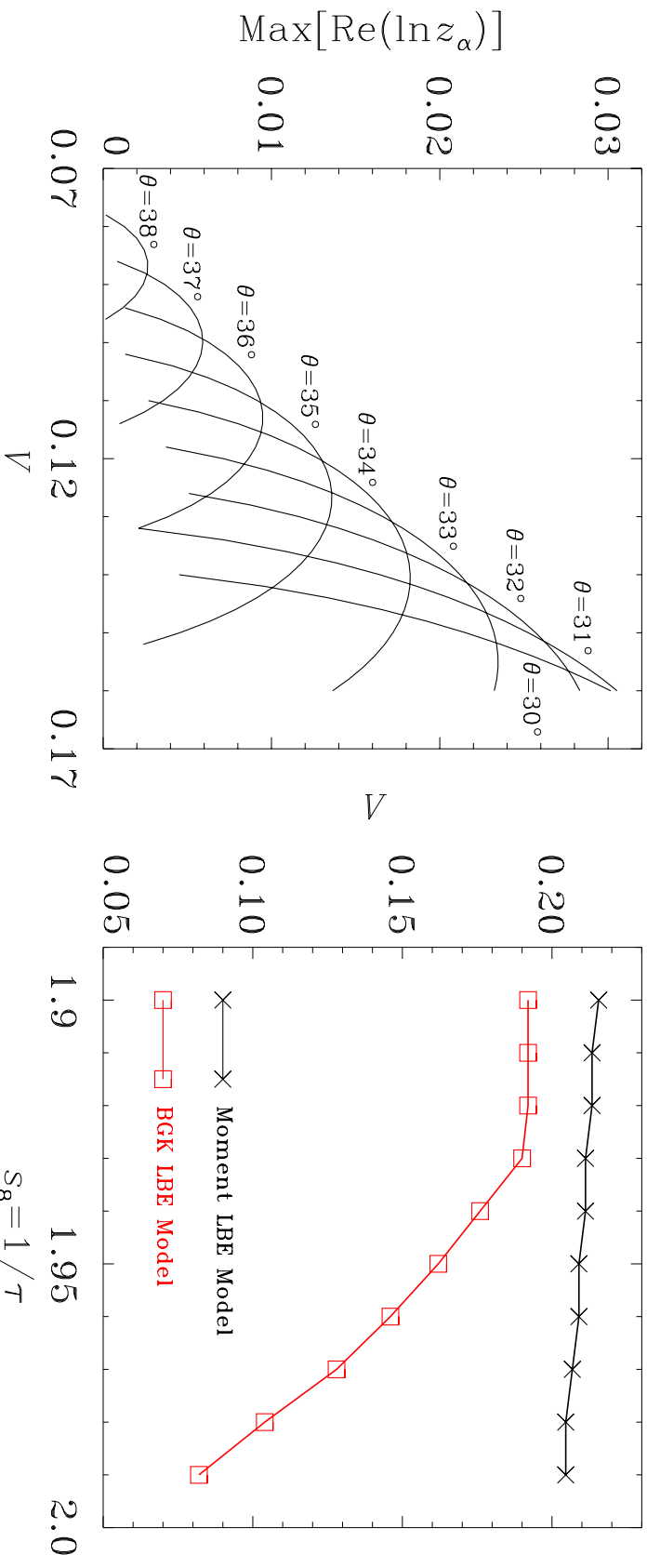
# Behaviors of Transport Coefficients



$k$  dependence of viscosities and  $g$ -factor. The solid lines, dotted lines, and dashed lines correspond to  $\theta = 0$ ,  $\pi/8$ , and  $\pi/4$ , respectively. LBE model (1) with no interpolation, (2) with central interpolation, and (3) with upwind interpolation.

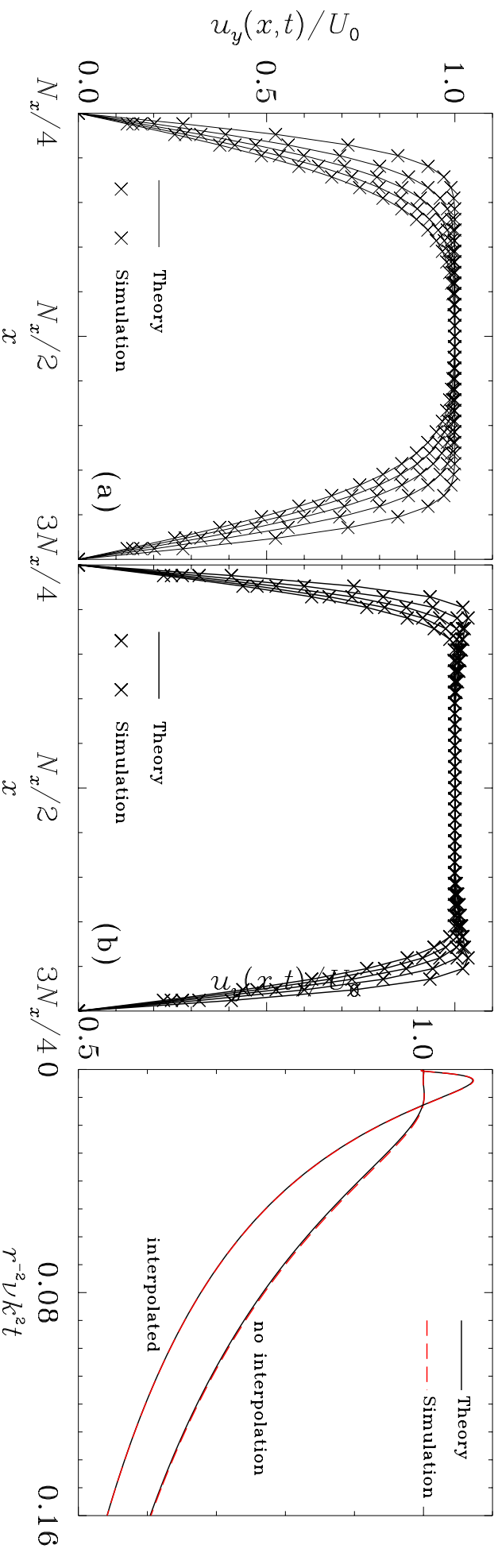
# Local Stability Analysis

If  $\text{Re}(\ln z_\alpha) > 0$ , mode  $|\varrho_\alpha\rangle$  is **unstable**.



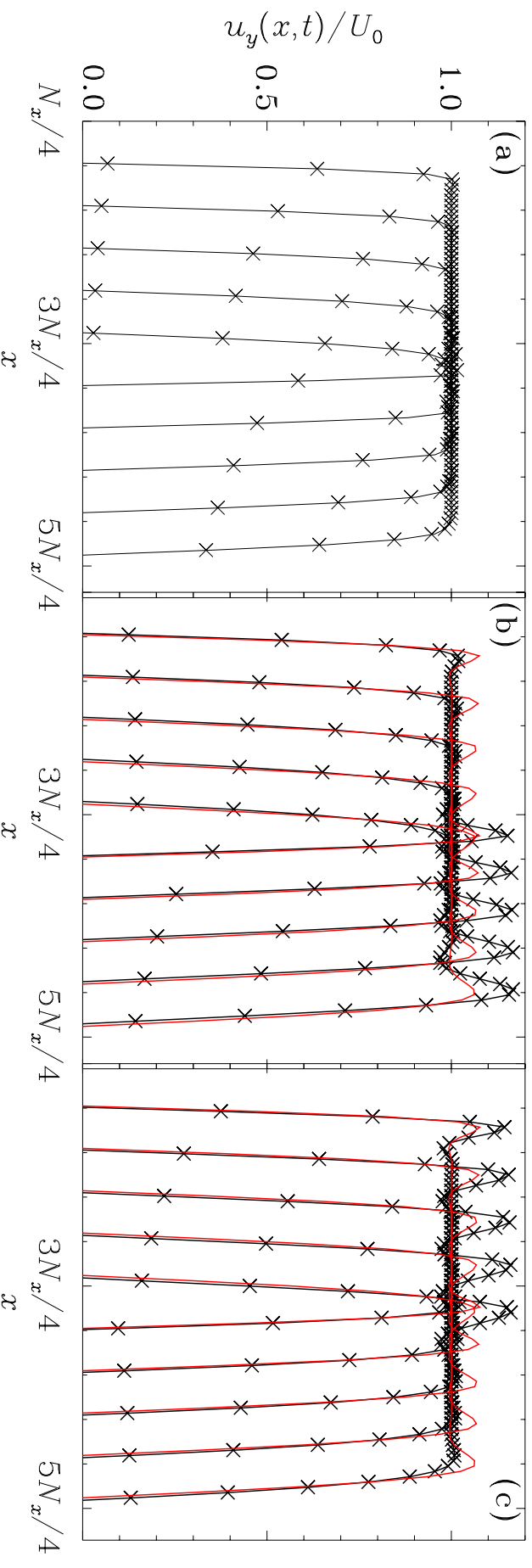
Stability of the generalized LBE model vs. the BGK LBE model in the parameter space of  $V$  and  $s_g = 1/\tau$ . (left)  $\text{max}[\text{Re}(\ln z_\alpha)]$  for given  $V$ . (right) Stability region of GLBE vs. LBGK model.

## Artifacts of the LBE Method



Decay of discontinuous shear wave velocity profile  $u_y(x, t)$ . The lines and symbols (X) are theoretical and numerical results, respectively. Only the positive half of each velocity and numerical profile is shown. LBE model (a) with no interpolation, (b) with the central interpolation and  $r = 0.5$ . (right) at a location close to the discontinuity  $x = 3N_x/4$ . The time is rescaled as  $r^{-2} \nu k^2 t$ .

## Artifacts of the LBE Method



Decay of discontinuous shear wave velocity profile  $u_y(x, t)$  with a constant streaming velocity  $V_x = 0.08 = U_0$ . The solid lines and symbols (X) are theoretical and numerical results, respectively. The dashed lines in (b) and (c) are obtained by setting  $g_n = 1$ . (a) no interpolation, (b) central interpolation and  $r = 0.5$ , (c) upwind interpolation and  $r = 0.5$ .

## Conclusions

- The Generalized LBE is superior than the Lattice BGK model;
- Analysis of the (linear) dispersion equation is equivalent to the Chapman-Enskog analysis, while Chapman-Enskog analysis is not valid for situation of finite wavevector  $k$ ;
- Analysis of the (linear) dispersion equation is also applicable to complex fluids (e.g., viscoelastic fluids).
- Limitations of the dispersion equation analysis:
  - Nonlocal effects (gradients);
  - Boundary conditions.