Lattice Boltzmann equations for higher-order partial differential equations

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17 April 2019

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Work conducted with François Dubois (Orsay) and Hiroshi Otomo (Tufts)

Outline

Chapman-Enskog expansion

- NS equations derive from Boltzmann equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \boldsymbol{\nabla} f = \Omega(f)$$

  - Knudsen number: $\mathrm{Kn} \sim \lambda/L \sim O(\epsilon)$
  - Mach number: $\mathrm{M} \sim u/c_s \sim O(\epsilon)$
  - Reynolds number: $\mathrm{Re} \sim \mathrm{M}/\mathrm{Kn} \sim O(1)$
- Hydrodynamic moments
  - Mass: $\rho = \int d\mathbf{v}\; mf$
  - Momentum: $\rho\mathbf{u} = \int d\mathbf{v}\; m\mathbf{v}f$
  - Pressure: $P = \int d\mathbf{v}\; m(\mathbf{v}-\mathbf{u})(\mathbf{v}-\mathbf{u})f$
- Satisfy incompressible Navier-Stokes equations

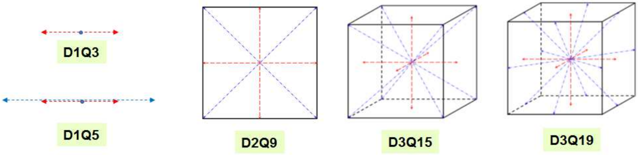
$$\boldsymbol{\nabla} \cdot \mathbf{u} = 0 \quad \text{and} \quad \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \boldsymbol{\nabla} \mathbf{u} = -\boldsymbol{\nabla} P + \nu \nabla^2 \mathbf{u}$$

Motivation for Kinetic Models of fluids

- Boltzmann equation (BE) lives in a bigger space:
  - Boltzmann: $f(\mathbf{x}, \mathbf{v}, t)$
  - Navier-Stokes: $\rho(\mathbf{x}, t)$, $\mathbf{u}(\mathbf{x}, t)$, and $P(\mathbf{x}, t)$
- Robustness:
  - BE more forgiving to radical discretization
  - CE expansion insensitive to form of collision operator
- More convenient to discretize:
  - BE equation is linear where it is nonlocal
  - BE equation is local where it is nonlinear
  - Upwind differencing not needed

Lattice Boltzmann models

- Benzi, Succi, Vergassola, *Phys. Rep.* **222** (1992)
- Discretization



  - Discrete velocity space: $\mathbf{c}_j$ for $j \in \{1, \ldots, b\}$ lie on lattice
  - Distribution function: $f_j(\mathbf{x}, t)$ for $j \in \{1, \ldots, b\}$
- Discrete kinetic equation

$$f_j(\mathbf{x} + \mathbf{c}_j, t + \Delta t) = f_j(\mathbf{x}, t) + \Omega_j\left(f\left(\mathbf{x}, t\right)\right)$$

- Conserved moments satisfy NS equations
  - Mass: $\rho = \sum_j f_j m_j$
  - Momentum: $\rho \mathbf{u} = \sum_j f_j m_j \mathbf{c}_j$
  - Pressure: $P = \sum_j f_j m_j (\mathbf{c}_j - \mathbf{u})(\mathbf{c}_j - \mathbf{u})$

Lattice BGK Model

- Qian, d'Humières, Lallemand, *Europhys. Lett.* **17** (1992)
- BGK collision operator with collisional relaxation time τ
- Distribution changes toward an equilibrium state, whose form determines the corresponding macroscopic equations,

$$\Omega_j\left(f\left(\mathbf{x},t\right)\right) = \frac{1}{\tau}\left[f_j^{\mathrm{eq}}\left(\mathbf{x},t\right) - f_j\left(\mathbf{x},t\right)\right]$$

- Demand f^{eq} has same hydrodynamic moments as f so collision operator respects conservation laws
- Viscosity $\nu \propto \left(\tau - 1/2\right)$

Local equilibrium distribution

- If the Maxwellian is employed for f_j^{eq}, LB equation, a governing equation in the LBM, leads to the Navier-Stokes equation with the Chapman-Enskog (CE) expansion

$$f_j^{eq} = \rho W_j \exp\left(-\frac{(\mathbf{c}_j - u)^2}{2T}\right) = \rho W_j \left\{1 + \frac{\mathbf{c}_j \cdot u}{T} + \left(\frac{(\mathbf{c}_j \cdot \mathbf{u})^2}{2T^2} - \frac{|\mathbf{u}|^2}{2T}\right) + \cdots\right\}$$

under the assumption of low Mach number, $\frac{|\mathbf{u}|}{\sqrt{T}} \ll 1$

- This form yields the Navier-Stokes equations

Example: 1D compressible NS equations

- 1DQ3 lattice
- Lattice vectors: $c_j = \{-1, 0, +1\}_j$
- Weights: $W_j = \{1/6, 2/3, 1/6\}_j$
- Isothermal: $T = 1/3$
- Second velocity moment: $\sum_j f_j^{\mathrm{eq}} |c_j|^2 = \rho T + \rho u^2$
- Resulting hydrodynamic equations:

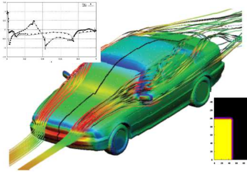
$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0$$
$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho u^2) = -T\frac{\partial \rho}{\partial x} + \nu \frac{\partial^2 u}{\partial x^2}$$

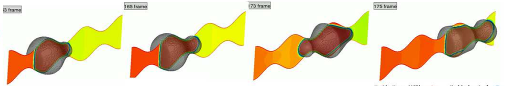
Contrast with more conventional numerical analysis

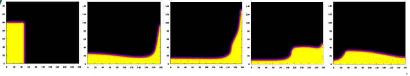
- Most numerical methods begin with PDEs for the desired quantities, and discretize to obtain a discrete dynamical system.
- LBEs begin with a physically motivated discrete dynamical system, endowed with conserved quantities, and figure out the hydrodynamic PDE obeyed by those quantities.
- With LBEs, the PDE "comes uninvited".
- Universality
- Inverse problem (posed by Succi): Given a system of PDEs, can we construct an LBE whose conserved quantities are governed by those PDEs?

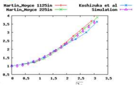
Pros and cons

- Algorithm is simple, fully explicit, easily parallelized
- Developed 25 years ago; commercialized software today
- More elaborate variations exist
  - Compressible flow
  - Irregular grids
  - Complex fluids
- Reduce τ to lower viscosity $\nu \propto (\tau - \frac{1}{2})$
  - Stable for $\tau \geq 1$ (underrelaxation)
  - Often unstable for $\frac{1}{2} < \tau < 1$ (overrelaxation)
  - Instability limits maximum Re attainable





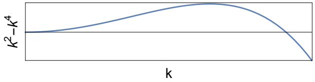




Kuramoto-Sivashinsky equation

- Introduce negative diffusion, regularized by hyper-diffusion.

$$\mathcal{F}(-h_{xx} - h_{xxxx}) = (k^2 - k^4)\mathcal{F}(h)$$



- KS equation is deterministic PDE,

$$\boxed{h_t + \frac{1}{2}h_x^2 = -h_{xx} - h_{xxxx}}$$

- Flame-front interface, liquid surface flowing down incline
- G.I. Sivashinsky, D.M. Michelson, "On Irregular Wavy Flow of a Liquid Film Down a Vertical Plane," **63** *Prog. Theor. Phys.* (1980) 2112-2114.

Dynamic universality class

- Dimensionless stochastic averages, such as $E[h^{2m}]/E[h^2]^m$ can be studied for both the KPZ and KS equations.
- For a particular noise variance β in the KPZ equation, these appear to be identical for all m.
- Conjecture: KS is in "KPZ universality class"
- In spite of fact that KS is deterministic and KPZ is stochastic
- Variance β is emergent
- References:
  - Conjecture: V. Yakhot, *Phys. Rev. A* **24** (1981) 642.
  - 1D numerical: S. Zaleski, *Physica D* **34** (1989) 427.
  - 2D numerical: BMB, C.C. Chow, T. Hwa, *Phys. Rev. Lett.* **83** (1999) 5262.

Prior work

- Existing work:
  - H. Lai, C. Ma, "Lattice boltzmann method for the generalized Kuramoto-Sivashinsky equation," *Physica A* **388** (2009)1405-1412.
  - L. Ye, G. Yan, T. Li, "Numerical method based on the lattice Boltzmann model for the Kuramoto-Sivashinsky equation," *J. Sci. Comput.*} **49** *(2011)195-210.*
- Motivation for current work:
  - Find simpler LBEs for KS equation
  - Find general methodology to assess accuracy of LBE, and find versions with higher accuracy
  - Find how to create LBE for more general higher-order PDES

Target PDEs for this study

- H. Otomo, B.M. Boghosian, F. Dubois, *Physica A* **486** (2017)
- One spatial dimension
- One scalar conserved quantity
- Examples:
  - Burgers': $\partial_t \rho + \rho \partial_x \rho = \partial_x^2 \rho$
  - Korteweg-de Vries (KdV): $\partial_t \rho - 6\rho \partial_x \rho = -\partial_x^3 \rho$
  - Kuramoto-Sivashinsky (KS): $\partial_t \rho + \rho \partial_x \rho = -\partial_x^2 \rho - \partial_x^4 \rho$

Chapman-Enskog method

- Lattice BGK equation
  - $f_j\left(x+c_j, t+\Delta t\right) - f_j\left(x, t\right) = -\frac{1}{\tau}\left[f_j\left(x, t\right) - f_j^{\mathrm{eq}}\left(x, t\right)\right]$
  - Here $\sum_j f_j^{\mathrm{eq}} = \sum_j f_j$ to conserve density
  - Define differential operator $D_j = \partial_t + c_j \partial_x$
  - $e^{D_j} f_j\left(x, t\right) - f_j\left(x, t\right) = -\frac{1}{\tau}\left[f_j\left(x, t\right) - f_j^{\mathrm{eq}}\left(x, t\right)\right]$

Formal solution to LB equation

$$f_j(x,t) = \left[1 + \tau\left(e^{D_j} - 1\right)\right]^{-1} f_j^{eq}(x,t)$$

Asymptotic ordering

- Time: $\partial_t = \sum_{k=1}^{\infty} \epsilon^k \partial_{t_k}$
- Space: $\partial_x = \epsilon \partial_{x_1}$
- Operator: $D_j = \sum_{k=0}^{\infty} \epsilon^k D_{j,k}$
- Distributions:
  - $f_j(\rho) = \sum_{k=0}^{\infty} \epsilon^k f_j^{(k)}$
  - $f_j^{eq}(\rho) = \sum_{k=0}^{\infty} \epsilon^k f_j^{(eq,k)}(\rho)$
  - $f_j^{(0)} = f_j^{(eq,0)}$

Chapman-Enskog method

- Result, after considerable algebra is

$$
\begin{aligned}
f_j^{(0)}(x,t) =& f_j^{(eq,0)} \\
f_j^{(1)}(x,t) =& -\tau D_{j,1} f_j^{(eq,0)} + f_j^{(eq,1)} \\
f_j^{(2)}(x,t) =& -\tau \left[D_{j,2} - \left(\tau - \tfrac{1}{2}\right) D_{j,1}^2 \right] f_j^{(eq,0)} - \tau D_{j,1} f_j^{(eq,1)} + f_j^{(eq,2)} \\
f_j^{(3)}(x,t) =& -\tau \left[D_{j,3} - 2\left(\tau - \tfrac{1}{2}\right) D_{j,1} D_{j,2} + \left(\tau^2 - \tau + \tfrac{1}{6}\right) D_{j,1}^3 \right] f_j^{(eq,0)} \\
& -\tau \left[D_{j,2} - \left(\tau - \tfrac{1}{2}\right) D_{j,1}^2 \right] f_j^{(eq,1)} - \tau D_{j,1} f_j^{(eq,2)} + f_j^{(eq,3)} \\
f_j^{(4)}(x,t) =& -\tau \left[D_{j,4} - 2\left(\tau - \tfrac{1}{2}\right) D_{j,1} D_{j,3} - \left(\tau - \tfrac{1}{2}\right) D_{j,2}^2 \right. \\
& \left. + 3\left(\tau^2 - \tau + \tfrac{1}{6}\right) D_{j,1}^2 D_{j,2} - \left(\tau - \tfrac{1}{2}\right)\left(\tau^2 - \tau + \tfrac{1}{12}\right) D_{j,1}^4 \right] f_j^{(eq,0)} \\
& -\tau \left[D_{j,3} - 2\left(\tau - \tfrac{1}{2}\right) D_{j,1} D_{j,2} + \left(\tau^2 - \tau + \tfrac{1}{6}\right) D_{j,1}^3 \right] f_j^{(eq,1)} \\
& -\tau \left[D_{j,2} - \left(\tau - \tfrac{1}{2}\right) D_{j,1}^2 \right] f_j^{(eq,2)} - \tau D_{j,1} f_j^{(eq,3)} + f_j^{(eq,4)}
\end{aligned}
$$

- Now sum LB equation over i at each order to obtain hydrodynamic equation for ρ

Moment definitions

- Moments are defined as follows

$$\begin{pmatrix} \rho \\ \mathcal{J}^{eq} \\ \mathcal{K}^{eq} \\ \mathcal{L}^{eq} \\ \mathcal{M}^{eq} \end{pmatrix} = \sum_j f_j^{eq} \begin{pmatrix} 1 \\ c_j \\ c_j^2 \\ c_j^3 \\ c_j^4 \end{pmatrix} = \sum_k \epsilon^k \begin{pmatrix} \rho_k^{eq} \\ J_k^{eq} \\ K_k^{eq} \\ L_k^{eq} \\ M_k^{eq} \end{pmatrix}$$

- where we have defined contributions at each order in ϵ

$$\begin{pmatrix} \rho_k^{eq} \\ J_k^{eq} \\ K_k^{eq} \\ L_k^{eq} \\ M_k^{eq} \end{pmatrix} = \sum_j f_j^{(eq,k)} \begin{pmatrix} 1 \\ c_j \\ c_j^2 \\ c_j^3 \\ c_j^4 \end{pmatrix},$$

- where $\rho_k^{eq} = \rho\, \delta_{k,0}$

Use of differing lattice weights at each order

- Equilibrium distribution function

$$f_j^{eq} = \rho w_j^{(0)} + \mathcal{J}^{eq} w_j^{(1)} + \mathcal{K}^{eq} w_j^{(2)} + \mathcal{L}^{eq} w_j^{(3)} + \mathcal{M}^{eq} w_j^{(4)}$$

- Example: D1Q5 lattice
  - Lattice vectors $c_j = \{-2, -1, 0, +1, +2\}_j$
  - Weights at each order

$$\begin{aligned}
w_j^{(0)} &= \{ \quad 0, \quad 0, \quad 1, \quad 0, \quad 0\}_j \\
w_j^{(1)} &= \{+1/12, -2/3, \quad 0, +2/3, -1/12\}_j \\
w_j^{(2)} &= \{-1/24, +2/3, -5/4, +2/3, -1/24\}_j \\
w_j^{(3)} &= \{-1/12, +1/6, \quad 0, -1/6, +1/12\}_j \\
w_j^{(4)} &= \{+1/24, -1/6, +1/4, -1/6, +1/24\}_j
\end{aligned}$$

Chapman-Enskog method

Table: Eqns. of motion and suppression conditions for each order in ϵ

ϵ order	Equations of motion	Conditions for $\partial_{t_j}\rho = 0$
1	$\partial_{t_1}\rho + J_0^{eq\prime}\,\partial_{x_1}\rho = 0$	$J_0^{eq\prime} = 0$
2	$\partial_{t_2}\rho = \partial_{x_1}\left\{\left(\tau - \frac{1}{2}\right) K_0^{eq\prime}\,\partial_{x_1}\rho\right\} - J_1^{eq\prime}\,\partial_{x_1}\rho$	$K_0^{eq\prime} = 0, \quad J_1^{eq\prime} = 0$
3	$\partial_{t_3}\rho = -\partial_{x_1}^2\left\{\left(\tau^2 - \tau + \frac{1}{6}\right) L_0^{eq\prime}\,\partial_{x_1}\rho\right\}$	$L_0^{eq\prime} = 0,$
	$+\left(\tau - \frac{1}{2}\right)\left(K_1^{eq\prime\prime}\left(\partial_{x_1}\rho\right)^2 + K_1^{eq\prime}\,\partial_{x_1}^2\rho\right) - J_2^{eq\prime}\,\partial_{x_1}\rho$	$K_1^{eq\prime} = 0, \quad J_2^{eq\prime} = 0$
4	$\partial_{t_4}\rho = \left(\tau - \frac{1}{2}\right)\left(\tau^2 - \tau + \frac{1}{12}\right)\partial_{x_1}^4 M_0^{eq}$ $-\left(\tau^2 - \tau + \frac{1}{6}\right)\partial_{x_1}^3 L_1^{eq} + \left(\tau - \frac{1}{2}\right)\partial_{x_1}^2 K_2^{eq} - \partial_{x_1} J_3$	

- For jth order, motions of kth order $(k < i)$ are suppressed.

Chapman-Enskog method

- Suppression conditions for example PDEs

Burgers'	$J_1^{eq} = \rho^2/2$	$K_0^{eq} = \frac{\rho}{\tau - 1/2}$		
KdV	$J_2^{eq} = -3\rho^2$	$K_1^{eq} = 0$	$L_0^{eq} = \frac{\rho}{\tau^2 - \tau + 1/6}$	
KS	$J_3^{eq} = \rho^2/2$	$K_2^{eq} = -\frac{\rho}{\tau - 1/2}$	$L_1^{eq} = 0$	$M_0^{eq} = -\frac{\rho}{(\tau - 1/2)\left(\tau^2 - \tau + 1/12\right)}$

Conversion to physical units

- Space and time in lattice units: $x = x_1$ and $t = t_p$
- Space and time in physical units: X and T
- Conversion factors
  - $X = \alpha x$
  - $T = \beta t$
- A typical choice

	Burgers'	KdV	KS
α	ϵ	ϵ	ϵ
β	ϵ^2	ϵ^3	ϵ^4

Equilibrium distribution

- Resulting contributions to equilibrium distribution:

	Burgers'	KdV	KS
$\mathcal{J}^{eq}$	$\frac{\beta\rho^2}{2\alpha}$	$-\frac{3\beta\rho^2}{\alpha}$	$\frac{\beta\rho^2}{2\alpha}$
$\mathcal{K}^{eq}$	$\frac{\rho\beta}{\alpha^2(\tau-1/2)}$	0	$-\frac{\beta\rho}{\alpha^2(\tau-1/2)}$
$\mathcal{L}^{eq}$	0	$\frac{\rho\beta}{\alpha^3\left(\tau^2-\tau+1/6\right)}$	0
$\mathcal{M}^{eq}$	0	0	$-\frac{\rho\beta}{\alpha^4(\tau-1/2)\left(\tau^2-\tau+1/12\right)}$

- Any τ yields same hydrodynamic equation at leading order

Comparisons with previous studies

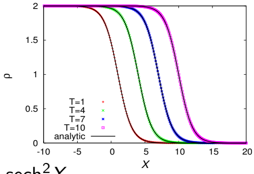
- In previous studies, HOLB models were derived using the Chapman-Enskog method
- Lai and Ma, *Physica A* **388** (2009)
  - Unphysical *amending function* introduced
  - Parameter ϵ assumed equal to timestep
- Chai, He, Guo, Shi, *Phys. Rev. E* **97** (2018)
  - Moments of equilibrium state chosen so p-th order PDE is $\partial_{t_p}\rho + \partial_{x_1}^p \left[\alpha_p F\left(\rho\right)\right] = 0$
  - HOPDEs derived by summing results at different orders, including powers of ϵ, i.e., $\partial_t = \epsilon\partial_{t_1} + \epsilon^2\partial_{t_2} + \epsilon^3\partial_{t_3} + \epsilon^4\partial_{t_4} + \cdots$
  - Procedure seems inconsistent with fundamental assumption of Chapman-Enskog method: Higher-order terms in ϵ are less important.
- In this study, above issues solved using suppression conditions

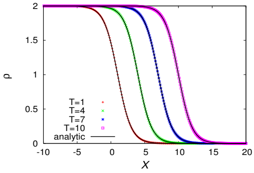
Numerical tests on Burgers' equation (top) & Korteweg-de Vries equation (bottom)

$\rho\,(X_M,t)=0,\;\; \rho\,(X_m,t)=2, \qquad \rho\,(X,0)=1-\;\tanh\left(\frac{X}{2}\right)$

$\rho\,(X,T)=1-\;\tanh\left(\frac{X-T}{2}\right)$

$\tau=1.25(\text{left}),\;\tau=1.5\;(\text{right}),\;\alpha=\Delta X=0.1,\;\beta=\Delta T=1.0e-3,\;\text{D1Q5}$

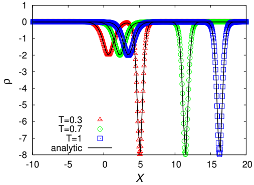


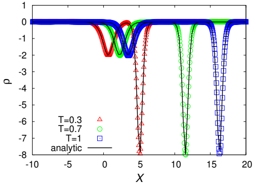


$\rho\,(X,0)=-6\;\text{sech}^2 X,$

$\rho\,(X,T)=-12\;\{3+4\;\cosh\,(2X-8T)+\cosh\,(4X-64T)\}\,/\left\{[3\;\cosh\,(X-28T)+\cosh\,(3X-36T)]^2\right\}$

$\tau=1.0(\text{left}),\;\tau=1.25\;(\text{right})\;,\;\alpha=\Delta X=0.05,\;\beta=\Delta T=2.5e-6,\;\text{D1Q7}$





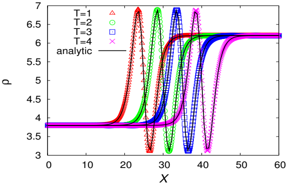
Numerical tests on Kuramoto-Sivashinsky equation

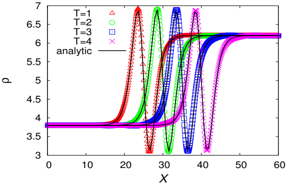
$$\rho\left(X_M,T\right)=b-\frac{30}{19}\sqrt{\frac{11}{19}},\ \ \rho\left(X_m,T\right)=2b-\rho\left(X_M,T\right),\ b=3,\ X_M=60,\ X_m=0$$

$$\rho\left(X,0\right)=b+\frac{15}{19}\sqrt{\frac{11}{19}}\left\{-9\tanh\left(k\left(X-X_0\right)\right)+11\tanh^3\left(k\left(X-X_0\right)\right)\right\},\ k=\frac{1}{2}\sqrt{\frac{11}{19}},\ X_0=\frac{X_M-X_m}{3}$$

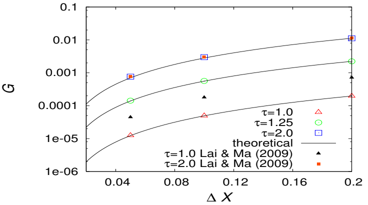
$$\rho(X,T)=b+\frac{15}{19}\sqrt{\frac{11}{19}}\left\{-9\tanh\left(k\left(X-bT-X_0\right)\right)+11\ \tanh^3\left(k\left(X-bT-X_0\right)\right)\right\}$$

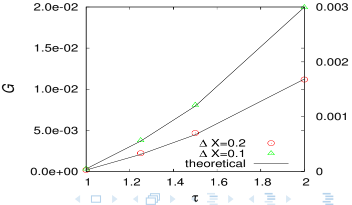
$\tau=1$ (left), $\tau=1.5$ (right), $\alpha=\Delta X=0.1$, $\beta=\Delta T=1.0\text{e-}5$, D1Q5





$$G:=\sum_x\left|\rho^N\left(x\right)-\rho^A\left(x\right)\right|/\sum_x\rho^A\left(x\right)$$





Enhanced HOLBM

- H. Otomo, BMB, F. Dubois, "Efficient lattice Boltzmann models for the Kuramoto-Sivashinsky equation," *Computers & Fluids* **172** (2018) 683-688.
- Through higher order analysis, modified f_j^{eq} for D1Q7 is derived

$$f_j^{eq} = \rho w_j^{(0)} + \mathcal{J}^{eq} w_j^{(1)} + \mathcal{K}^{eq} w_j^{(2)} + \left(\mathcal{M}^{eq} + \delta\mathcal{M}^{eq}\right) w_j^{(4)} + \frac{120\rho(\mathcal{T}_1+1)\beta}{(\mathcal{T}_4+1)\alpha^4} w_j^{(6)}$$

$$\delta\mathcal{M}^{eq} = -\frac{24\rho\beta^2(\mathcal{T}_1+1)}{\alpha^4(\mathcal{T}_4+1)}\left(\frac{\mathcal{T}_2+1}{2(\mathcal{T}_1+1)} - \frac{\mathcal{T}_3+1}{\mathcal{T}_4+1}\right), \quad \mathcal{T}_i = \sum_{n=1}^{\infty}\left(1-\frac{1}{\tau}\right)^n\left[(n+1)^i - n^i\right]$$

$$w_j^{(6)} = \left\{-\frac{1}{36}, \frac{1}{48}, -\frac{1}{120}, \frac{1}{720}\right\}_j$$

- Using this f_j^{eq}, relaxation time, and D1Q7, the same accuracy level is achieved with larger time increments compared to original D1Q5 scheme. As a result, computational costs are saved by 90%

Discussion

- It is necessary to suppress the motion at each order, in order for that at the next order to be visible in the asymptotic limit.
- We have effectively solved Succi's "inverse Chapman-Enskog" problem for one spatial dimension, and one scalar conserved quantity, including acoustiv, diffusive, and hyperdiffusive scaling.
- Natural generalizations are
  - higher spatial dimensions
  - more conserved quantities.

Acknowledgements

- Thanks to the Fondation Mathématique Jacques Hadamard (FMJH)
- Thank you for your attention!