Lattice Boltzmann Equations and Finite-Difference Schemes

Dominique d'Humières [1] Irina Ginzburg [2]

[1]Laboratoire de Physique Statistique,
École Normale Supérieure

[2]Cemagref, Antony Regional Centre, HBAN

December 5, 2008

Outline

LB models.
General framework.

- a cubic lattice in D dimensions,
- a set of Q velocities $(\vec{c}_q \delta x / \delta t)$ connecting nodes of the lattice and such that, for any $\vec{c}_q$ in the set, $\vec{c}_{\bar{q}} = -\vec{c}_q$ is also in the set,
- an associated set of particle densities $f_q(\vec{r}, t)$ $(\mathbf{f} = (f_q))$,
- an evolution equation for these particle densities:

$$f_q(\vec{r} + \vec{c}_q \delta x, t + \delta t) = f_q^*(\vec{r}, t) \equiv f_q(\vec{r}, t) + \mathcal{C}_q(\mathbf{f}(\vec{r}, t)),$$

where $\mathcal{C}$ is a collision term function of $\mathbf{f}$.

LB models.

Some velocity sets.

- D1Q3: $\{-1, 0, 1\}$,
- D2Q5: $\{(0, -1), (-1, 0), (0, 0), (1, 0), (0, 1)\}$,
- D2Q9: D2Q5 $\cup \{(-1, -1), (-1, 1), (1, -1), (1, 1)\}$,
- D3Q7: $\{(0, 0, 0), (\pm 1, 0, 0), (0, \pm 1, 0), (0, 0, \pm 1)\}$,
- D3Q9: $\{(0, 0, 0), (\pm 1, \pm 1, \pm 1)\}$,
- D3Q13: $\{(0, 0, 0), (\pm 1, \pm 1, 0), (\pm 1, 0, \pm 1), (0, \pm 1, \pm 1)\}$,
- D3Q15: D3Q7 $\cup$ D3Q9,
- D3Q19: D3Q7 $\cup$ D3Q13,
- D3Q27: D3Q7 $\cup$ D3Q9 $\cup$ D3Q13,

LB models.

Collisions through relaxation.

Following Higuera et al. (1989), the collision term is done through a relaxation toward a given “attractor” **e** function of **f**: $\mathcal{C}(\mathbf{f}) = -\mathcal{A} \cdot (\mathbf{f} - \mathbf{e}(\mathbf{f}))$, where $\mathcal{A}$ is a given collision operator.

- BGK (Bhatnagar-Gross-Krook) or SRT (Single-Relaxation-Time): $\mathcal{A} = \lambda \mathcal{I}$ $(\lambda = 1/\tau)$.
- MRT (Multiple-Relaxation-Time): $\mathcal{A}$ is defined by its eigenvalues (relaxation times) and its eigenvectors.
  - “Kinetic” models: eigenvectors based on the velocity set, $\mathbf{b}_{mnp} = (c_{qx}^m c_{qy}^n c_{qz}^p)$.
  - L-models (I. Ginzburg): based on the symmetric and antisymmetric components of **f**.

LB models.
Two-Relaxation-Time (TRT) LBE.

Splitting the particle densities in their symmetric and antisymmetric components:

$$f_q^+ = \frac{(f_q + f_{\bar q})}{2}, \qquad f_q^- = \frac{(f_q - f_{\bar q})}{2},$$
$$f_q = f_q^+ + f_q^-, \qquad f_{\bar q} = f_q^+ - f_q^-.$$

the TRT evolution is given by

$$f_q(\vec r + \vec c_q \delta x, t + \delta t) = [f_q - \lambda^+ (f_q^+ - e_q^+) - \lambda^- (f_q^- - e_q^-)](\vec r, t),$$

or with $\lambda^* = (\lambda^+ + \lambda^-)/2$ and $\delta\lambda = (\lambda^+ - \lambda^-)/2$

$$f_q(\vec r + \vec c_q \delta x, t + \delta t) = [(1 - \lambda^*) f_q - \delta\lambda\, f_{\bar q} + \lambda^* e_q + \delta\lambda\, e_{\bar q}](\vec r, t),$$

LB models.
Conserved quantities

The fundamental ingredient of the LB models is the existence of quantities conserved during the collision, for instance the mass:

$$\rho = \sum_q f_q = \sum_q f_q^*,$$

the momentum

$$\rho\vec{u} = \sum_q f_q \vec{c}_q = \sum_q f_q^* \vec{c}_q,$$

energy ...

LB models.
Conserved quantities

The fundamental ingredient of the LB models is the existence of quantities conserved during the collision, for instance the mass:

$$\rho = \sum_q f_q = \sum_q f_q^*,$$

the momentum

$$\rho\vec{u} = \sum_q f_q \vec{c}_q = \sum_q f_q^* \vec{c}_q,$$

energy ...

LB models.
Conserved quantities

The fundamental ingredient of the LB models is the existence of quantities conserved during the collision, for instance the mass:

$$\rho = \sum_q f_q = \sum_q f_q^*,$$

the momentum

$$\rho \vec{u} = \sum_q f_q \vec{c}_q = \sum_q f_q^* \vec{c}_q,$$

energy ...

LB models.
equilibrium

The "attractor" of the relaxation (also called equilibrium) is restricted to be functions of the conserved quantities only. To satisfy the conservation laws, the equilibrium must be chosen such that:

$$\sum_q e_q = \rho,$$

for the mass,

$$\sum_q e_q \vec{c}_q = \rho \vec{u}.$$

for the momentum ...

LB models.

equilibrium

The “attractor” of the relaxation (also called equilibrium) is restricted to be functions of the conserved quantities only. To satisfy the conservation laws, the equilibrium must be chosen such that:

$$\sum_q e_q = \rho,$$

for the mass,

$$\sum_q e_q \vec{c}_q = \rho \vec{u}.$$

for the momentum ...

von Neumann stability.

In a periodic domain, the solutions of the linearized evolution equations have the form:

$$\mathbf{f}(\vec{r}, t) = \Omega^{t/\delta t} \exp(i\vec{k} \cdot \vec{r}/\delta x)\mathbf{f}_0,$$

The population **f** after advection is given by

$$\mathbf{f}(\vec{r} + \vec{c}_q \delta x, t + \delta t) = \Omega e^{k_q} \mathbf{f}(\vec{r}, t),$$

with $\vec{k} \cdot \vec{c}_q$. Using $\mathcal{K} = \mathrm{diag}(e^{k_q})$ and $\mathbf{e} = \mathcal{E}\mathbf{f}$, it comes

$$(\mathcal{I} - \mathcal{A} \cdot (\mathcal{I} - \mathcal{E})) \cdot \mathbf{f}_0 = \Omega \mathcal{K} \cdot \mathbf{f}_0.$$

von Neumann stability.

Writing the system:

$$\Omega\, \mathbf{f}_0 = \mathcal{K}^{-1} \cdot (\mathcal{I} - \mathcal{A} \cdot (\mathcal{I} - \mathcal{E})) \cdot \mathbf{f}_0,$$

the growth rate Ω can take one of the eigenvalue of the matrix $\mathcal{K}^{-1} \cdot (\mathcal{I} - \mathcal{A} \cdot (\mathcal{I} - \mathcal{E}))$.
The LB model will be stable for a set of parameters defining $\mathcal{A}$ and $\mathcal{E}$ iff all the Ω are $|\Omega| \leq 1$ for all the values of $\vec{k}$ ($0 \leq \vec{k} \leq \pi$).

BGK model for $\lambda = 1$.

Finite-difference equivalent scheme.

For the BGK models the evolution equation is given by

$$f_q(\vec{r} + \vec{c}_q \delta x, t + \delta t) = [f_q - \lambda(f_q - e_q)](\vec{r}, t),$$

For $\lambda = 1$ this equation becomes

$$f_q(\vec{r} + \vec{c}_q \delta x, t + \delta t) = e_q(\vec{r}, t),$$

or

$$f_q(\vec{r}, t + \delta t) = e_q(\vec{r} - \vec{c}_q \delta x, t),$$

Projecting this equation on the conserved quantities, it comes

$$\rho(\vec{r}, t + \delta t) - \rho(\vec{r}, t) = \sum_q (e_q(\vec{r} - \vec{c}_q \delta x, t) - e_q(\vec{r}, t)),$$

BGK model for $\lambda = 1$.

Stability condition for $\lambda^* = 1$.

For models with only mass conservation (advection-diffusion), the linearized equilibrium can be written: $e_q = E_q \rho$, with $\sum_q E_q = 1$. The growth rate Ω is solution of

$$\Omega = \sum_q e_q e^{-k_q} = A + iB,$$

with

$$A = \sum_q E_q^+ \cos(k_q), \qquad B = \sum_q E_q^- \sin(k_q).$$

It can be shown that for any value of $\delta\lambda \in [-1, 1]$, $|\Omega| \leq 1$ iff $A^2 + B^2 \leq 1$.

Co-BGK LBE.

Evolution equation for $\lambda^* = 1$.

The TRT evolution equation is given by

$$f_q(\vec{r} + \vec{c}_q \delta x, t + \delta t) = [(1 - \lambda^*) f_q - \delta\lambda \, f_{\bar{q}} + \lambda^* e_q + \delta\lambda \, e_{\bar{q}}](\vec{r}, t),$$

Co-BGK LBE.

Evolution equation for $\lambda^* = 1$.

For $\lambda^* = 1$ the TRT evolution equation becomes

$$f_q(\vec{r} + \vec{c}_q \delta x, t + \delta t) = [-\delta\lambda \, f_{\bar{q}} + e_q + \delta\lambda \, e_{\bar{q}}](\vec{r}, t),$$

Co-BGK LBE.

Evolution equation for $\lambda^* = 1$.

For $\lambda^* = 1$ the TRT evolution equation can also be written

$$f_q(\vec{r}, t + \delta t) = [-\delta\lambda\, f_{\bar{q}} + e_q + \delta\lambda\, e_{\bar{q}}](\vec{r} - \vec{c}_q \delta x, t),$$

Co-BGK LBE.

Evolution equation for $\lambda^* = 1$.

For $\lambda^* = 1$ the TRT evolution equation can also be written

$$f_q(\vec{r}, t + \delta t) = [-\delta\lambda\, f_{\bar{q}} + e_q + \delta\lambda\, e_{\bar{q}}](\vec{r} - \vec{c}_q \delta x, t),$$

or

$$f_{\bar{q}}(\vec{r} - \vec{c}_q \delta x, t) = [-\delta\lambda\, f_q + e_{\bar{q}} + \delta\lambda\, e_q](\vec{r}, t - \delta t),$$

Co-BGK LBE.

Evolution equation for $\lambda^* = 1$.

For $\lambda^* = 1$ the TRT evolution equation can also be written

$$f_q(\vec{r}, t + \delta t) = [-\delta\lambda\, f_{\bar{q}} + e_q + \delta\lambda\, e_{\bar{q}}](\vec{r} - \vec{c}_q \delta x, t),$$

or

$$f_{\bar{q}}(\vec{r} - \vec{c}_q \delta x, t) = [-\delta\lambda\, f_q + e_{\bar{q}} + \delta\lambda\, e_q](\vec{r}, t - \delta t),$$

then

$$\begin{aligned} f_q(\vec{r}, t + \delta t) &= [e_q + \delta\lambda\, e_{\bar{q}}](\vec{r} - \vec{c}_q \delta x, t) \\ &- \delta\lambda\, [-\delta\lambda\, f_q + e_{\bar{q}} + \delta\lambda\, e_q](\vec{r}, t - \delta t), \end{aligned}$$

Co-BGK LBE.
Evolution equation for $\lambda^* = 1$.

Summing over q the equation

$$\begin{aligned} f_q(\vec{r}, t+\delta t) &= [e_q + \delta\lambda\, e_{\bar{q}}](\vec{r} - \vec{c}_q \delta x, t) \\ &- \delta\lambda\, [-\delta\lambda\, f_q + e_{\bar{q}} + \delta\lambda\, e_q](\vec{r}, t-\delta t), \end{aligned}$$

gives

$$\begin{aligned} \rho(\vec{r}, t+\delta t) &= \sum_q [e_q + \delta\lambda\, e_{\bar{q}}](\vec{r} - \vec{c}_q \delta x, t) \\ &- \delta\lambda \sum_q [-\delta\lambda\, f_q + e_{\bar{q}} + \delta\lambda\, e_q](\vec{r}, t-\delta t), \end{aligned}$$

Co-BGK LBE.

Evolution equation for $\lambda^* = 1$.

Summing over q the equation

$$\begin{aligned} f_q(\vec{r}, t+\delta t) &= [e_q + \delta\lambda\, e_{\bar{q}}](\vec{r} - \vec{c}_q \delta x, t) \\ &- \delta\lambda\, [-\delta\lambda\, f_q + e_{\bar{q}} + \delta\lambda\, e_q](\vec{r}, t-\delta t), \end{aligned}$$

gives also

$$\rho(\vec{r}, t+\delta t) = -\delta\lambda\, \rho(\vec{r}, t-\delta t) + \sum_q [e_q + \delta\lambda\, e_{\bar{q}}](\vec{r} - \vec{c}_q \delta x, t),$$

Co-BGK LBE.

Evolution equation for $\lambda^* = 1$.

Summing over q the equation

$$\begin{aligned} f_q(\vec{r}, t+\delta t) &= [e_q + \delta\lambda\, e_{\bar{q}}](\vec{r} - \vec{c}_q \delta x, t) \\ &- \delta\lambda\, [-\delta\lambda\, f_q + e_{\bar{q}} + \delta\lambda\, e_q](\vec{r}, t - \delta t), \end{aligned}$$

gives also

$$\begin{aligned} \rho(\vec{r}, t+\delta t) &= -\delta\lambda\, \rho(\vec{r}, t - dt) \\ &+ \sum_q [(1+\delta\lambda)e_q^+ + (1-\delta\lambda)e_q^-](\vec{r} - \vec{c}_q \delta x, t), \end{aligned}$$

Co-BGK LBE.

Evolution equation for $\lambda^* = 1$.

Summing over q the equation

$$
\begin{aligned}
f_q(\vec{r}, t+\delta t) &= [e_q + \delta\lambda\, e_{\bar{q}}](\vec{r} - \vec{c}_q \delta x, t) \\
&- \delta\lambda\, [-\delta\lambda\, f_q + e_{\bar{q}} + \delta\lambda\, e_q](\vec{r}, t-\delta t),
\end{aligned}
$$

gives finally a du Fort-Frankel scheme $((1+\delta\lambda)/(1-\delta\lambda) = 2\Lambda^-)$

$$
\frac{1}{2}(\rho(\vec{r}, t+\delta t) - \rho(\vec{r}, t-\delta t)) - \sum_q e_q^-(\vec{r} - \vec{c}_q \delta x, t) =
$$

$$
2\Lambda^- \sum_q (e_q^+(\vec{r} - \vec{c}_q \delta x, t) - \frac{1}{2}(e_q^+(\vec{r}, t+\delta t) + e_q^+(\vec{r}, t-\delta t))),
$$

Co-BGK LBE.

Stability condition for $\lambda^* = 1$.

The growth rate Ω is solution of

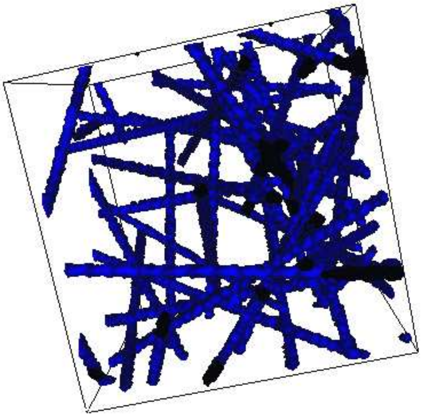
$$\Omega^2 - ((1 + \delta\lambda)A + i(1 - \delta\lambda)B)\Omega + \delta\lambda = 0,$$

with

$$A = \sum_q E_q^+ \cos(k_q), \qquad B = \sum_q E_q^- \sin(k_q).$$

It can be shown that for any value of $\delta\lambda \in [-1, 1]$, $|\Omega| \leq 1$ iff $A^2 + B^2 \leq 1$ as for BGK and $\tau = 1$.

Permeability of a porous medium.
Picture.



Permeability of a porous medium.
Table.

ν	λ_ν	50^3, $\phi \approx 0.973$	
		k_{xx}	
1/6	1	42.249358	
		$k^{\rm rel}$	
		$\Lambda^2 = 1/4$ (10^{-12})	*BGK*
1/24	8/5	0.1	−0.094
1/6	1	0	0.021
1/2	1/2	1.1	0.356
7/6	1/4	−0.3	1.123
5/2	1/8	0.3	2.946

Steady Recurrence Equations

Populations.

$$
\begin{aligned}
f_q(\vec{r}, t) &= [e_q^+ + e_q^- - (\frac{1}{2} + \Lambda^+) g_q^+ - (\frac{1}{2} + \Lambda^-) g_q^-](\vec{r}, t), \\
f_q^*(\vec{r}, t) &= [e_q^+ + e_q^- + (\frac{1}{2} - \Lambda^+) g_q^+ + (\frac{1}{2} - \Lambda^-) g_q^-](\vec{r}, t) \\
\Lambda^+ &= (\frac{1}{\lambda^+} - \frac{1}{2}) > 0 \,, \; \Lambda^- = (\frac{1}{\lambda^-} - \frac{1}{2}) > 0 \,, \; \forall\, q \,.
\end{aligned}
$$

Steady Recurrence Equations

Recurrence equations.

With the help of the following link-wise finite-difference operators,

$$\begin{aligned} \bar{\Delta}_q \phi(\vec{r}) &= \frac{1}{2}(\phi(\vec{r} + \vec{c}_q \delta x) - \phi(\vec{r} - \vec{c}_q \delta x)), \\ \Delta_q^2 \phi(\vec{r}) &= \phi(\vec{r} + \vec{c}_q \delta x) - 2\phi(\vec{r}) + \phi(\vec{r} - \vec{c}_q \delta x), \end{aligned}$$

and $\Lambda_q^{\mp} = \Lambda^+ \Lambda^-$, the steady evolution equation gives

$$\begin{aligned} g_q^{\pm}(\vec{r}) &= [\bar{\Delta}_q e_q^{\mp} - \Lambda_q^{\mp} \Delta_q^2 e_q^{\pm} + (\Lambda^2 - \frac{1}{4})\Delta_q^2 g_q^{\pm}](\vec{r}), \\ 0 &= [\Delta_q^2 e_q^{\pm} - \Lambda_q^{\pm} \Delta_q^2 g_q^{\pm} - \bar{\Delta}_q g_q^{\mp}](\vec{r}). \end{aligned}$$

Steady Recurrence Equations

Populations.

$$
\begin{aligned}
(\Lambda^+ g_q^+)(\vec{r}) &= [\bar{\Delta}_q(\Lambda^+ e_q^-) - \Lambda^2 \Delta_q^2 e_q^+ + (\Lambda^2 - \frac{1}{4})\Delta_q^2(\Lambda^+ g_q^+)](\vec{r}), \\
g_q^-(\vec{r}) &= [\bar{\Delta}_q e_q^+ - \Delta_q^2(\Lambda^+ e_q^-) + (\Lambda^2 - \frac{1}{4})\Delta_q^2 g_q^-](\vec{r}), \\
0 &= [\Delta_q^2 e_q^+ - \Delta_q^2(\Lambda^+ g_q^+) - \bar{\Delta}_q g_q^-](\vec{r}), \\
0 &= [\Delta_q^2(\Lambda^+ e_q^-) - \Lambda^2 g_q^- - \bar{\Delta}_q(\Lambda^+ g_q^+)](\vec{r}).
\end{aligned}
$$

Bounce-back rule, $f_{\bar{q}} = f_q^*$, gives $\Lambda^2 g_q^- = (\Lambda^+ e_q^-) + (\Lambda^+ g_q^+)/2$.

Summary

- Some LBEs are finite-difference schemes.
- The known results for convergence, stability, consistency apply for this class of LBE.
- For suitable boundary conditions, the steady state of TRT models is controlled by the product $\Lambda^+\Lambda^-$.

- Outlook
  - Have we found all the LBEs being FD schemes?
  - If it exists a class of LBE not being a FD scheme, does it change the LBE properties?
  - Can we get more analytic stability results?

Summary

- Some LBEs are finite-difference schemes.
- The known results for convergence, stability, consistency apply for this class of LBE.
- For suitable boundary conditions, the steady state of TRT models is controlled by the product $\Lambda^+\Lambda^-$.
- Outlook
  - Have we found all the LBEs being FD schemes?
  - If it exists a class of LBE not being a FD scheme, does it change the LBE properties?
  - Can we get more analytic stability results?

Summary

- Some LBEs are finite-difference schemes.
- The known results for convergence, stability, consistency apply for this class of LBE.
- For suitable boundary conditions, the steady state of TRT models is controlled by the product $\Lambda^{+}\Lambda^{-}$.

- Outlook
  - Have we found all the LBEs being FD schemes?
  - If it exists a class of LBE not being a FD scheme, does it change the LBE properties?
  - Can we get more analytic stability results?

Summary

- Some LBEs are finite-difference schemes.
- The known results for convergence, stability, consistency apply for this class of LBE.
- For suitable boundary conditions, the steady state of TRT models is controlled by the product $\Lambda^+\Lambda^-$.

- Outlook
  - Have we found all the LBEs being FD schemes?
  - If it exists a class of LBE not being a FD scheme, does it change the LBE properties?
  - Can we get more analytic stability results?

Summary

- Some LBEs are finite-difference schemes.
- The known results for convergence, stability, consistency apply for this class of LBE.
- For suitable boundary conditions, the steady state of TRT models is controlled by the product $\Lambda^+\Lambda^-$.

- Outlook
  - Have we found all the LBEs being FD schemes?
  - If it exists a class of LBE not being a FD scheme, does it change the LBE properties?
  - Can we get more analytic stability results?

Summary

- Some LBEs are finite-difference schemes.
- The known results for convergence, stability, consistency apply for this class of LBE.
- For suitable boundary conditions, the steady state of TRT models is controlled by the product $\Lambda^{+}\Lambda^{-}$.

- Outlook
  - Have we found all the LBEs being FD schemes?
  - If it exists a class of LBE not being a FD scheme, does it change the LBE properties?
  - Can we get more analytic stability results?