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Some elements of Lattice Boltzmann method for hydrodynamic and anisotropic advection-diffusion problems



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- U. Frisch, D. d'Humières, B. Hasslacher, P. Lallemand,
 Y. Pomeau, and J.P. Rivet, Lattice gas hydrodynamics in two and three dimensions., Complex Sys., 1, 1987
- F. J. Higuera and J. Jiménez, Boltzmann approach to lattice gas simulations. Europhys. Lett., 9, 1989
- D. d'Humières, Generalized Lattice-Boltzmann Equations, AIAA Rarefied Gas Dynamics: Theory and Simulations, 59, 1992
 - D. d'Humières, I. Ginzburg, M. Krafczyk, P. Lallemand and L.-S. Luo, Multiple-relaxation-time lattice Boltzmann models in three dimensions, Phil. Trans. R. Soc. Lond. A 360, 2005
 - I. Ginzburg, Equilibrium-type and Link-type Lattice Boltzmann models for generic advection and anisotropic-dispersion equation, Adv Water Resour, 28, 2005

Lattice Boltzmann two phase calculations in porous media, 2002 Fraunhofer Institut for Industrial Mathematics (ITWM), Kaiserslautern

Oil distribution in an anisotropic fibrous material

Fleece



oil is wetting



oil is non-wetting





Free surface Lattice Boltzmann method for Newtonian and Bingham fluid





I. Ginzburg and K. Steiner, Lattice Bolzmann model for free-surface flow and its application to filling process in casting, **J.Comp.Phys.**, **185**, **2003**

Key points

Basic LB method:

- (1) Linear collision operators
- (2) Chapman-Enskog expansion

Applications:

- Permeability computations in porous media (4)
- Richard's equations for variably saturated flow in heterogeneous anisotropic aquifers
- (3) Boundary schemes
 - Finite-difference type recurrence equations
- (5) Knudsen layers
- (6) Stability conditions
- (7) Interface analysis

Cubic velocity sets $\{\vec{c}_q, \quad q=0,\ldots,Q-1\}$ $\vec{c}_q=\{c_{q\alpha}\ ,\ \alpha=1,\ldots,d\}$ – d2Q5: $\vec{0}$ and

d2Q9



one rest (immobile): $\vec{c}_0 = \vec{0} = (0,0)$ $\mathbf{Q} - \mathbf{1}$ moving: $\vec{c}_q = (\pm 1,0), (0,\pm 1), (\pm 1,\pm 1)$ - d3Q7: $\vec{0}$ and $(\pm 1, 0, 0)$, $(0, \pm 1, 0)$, $(0, 0, \pm 1)$

 $(\pm 1,0), (0,\pm 1)$

- $d3Q13:\vec{0}$ and $(\pm 1,\pm 1,0), (0,\pm 1,\pm 1), (\pm 1,0,\pm 1)$
- $d3Q15:\vec{0}$ and (±1,0,0), (0,±1,0), (0,0,±1), (±1,±1,±1)
- $d3Q19: \vec{0} and$ (±1,0,0), (0,±1,0), (0,0,±1), (±1,±1,0), (0,±1,±1), (±1,0,±1)
- $d3Q27 = d3Q19 \cup d3Q15$

Multiple-relaxation-time MRT-model

Veloc	ity space	Moment space		
f_0	\vec{c}_0	\widehat{f}_0	\mathbf{b}_1	
f_k	\vec{c}_k	\widehat{f}_k	\mathbf{b}_k	
f_{Q-1}	\vec{c}_{Q-1}	$\widehat{f_{Q-1}}$	\mathbf{b}_{Q-1}	

- Moment (physical) space: basis vectors \mathbf{b}_k and eigenvalues λ_k , $k = 0, \dots, Q - 1.$
- Projection into moment space: $\mathbf{f} = \sum_{k=0}^{Q-1} \widehat{f}_k \mathbf{b}_k, \ \widehat{f}_k = \langle f | \mathbf{b}_k \rangle.$
- Collision in moment space: $[\mathcal{A} \cdot (\mathbf{f} - \mathbf{e})]_q =$ $\sum_{k=0}^{Q-1} \lambda_k (\widehat{f}_k - \widehat{e}_k) b_{kq}.$
- Linear stability: $-2 < \lambda_k < 0$.

Grid space:
$$\Delta r_{\alpha} = 1, \, \alpha = 1, \ldots, d$$

 $\Delta t = 1$ (1 update) Time:

- Population vector: $\mathbf{f}(\vec{r},t) = (f_q), \quad q = 0,..,Q-1$
- Equilibrium function: $\mathbf{e}(\vec{r},t) = (e_q), \quad q = 0,..,Q-1$
- $Collision_q(\vec{r},t) = [\mathcal{A} \cdot (\mathbf{f} \mathbf{e})]_q, \mathcal{A}[Q \times Q]$ -matrix $\tilde{f}_{a}(\vec{r},t) = f_{a}(\vec{r},t) + Collision_{a}$
- Propagation: $f_q(\vec{r} + \vec{c}_q, t+1) = \tilde{f}_q(\vec{r}, t)$

MRT basis of d2Q9 model

 $d2Q9: \mathbf{b}_k, k = 1, \dots, 9$

 $(\mathbf{b}_1)_q = \mathbf{1}$ $(\mathbf{b}_2)_q = c_{qx}$ $(\mathbf{b}_3)_q = c_{qy}$ $(\mathbf{b}_4)_q = 3c_q^2 - 4, c_q^2 = c_{qx}^2 + c_{qy}^2$ $(\mathbf{b}_5)_q = 2c_{qx}^2 - c_q^2$ $(\mathbf{b}_6)_q = c_{qx}c_{qy}$ $(\mathbf{b}_7)_q = c_{qx}(3c_q^2 - 5)$ $(\mathbf{b}_8)_q = c_{qy}(3c_q^2 - 5)$ $(\mathbf{b}_9)_q = \frac{1}{2}(9c_q^4 - 21c_q^2 + 8).$

b ₁	b ₂	b ₃	b ₄	b ₅	b ₆	b ₇	b ₈	b 9
1	0	0	-4	0	0	0	0	4
1	1	0	-1	1	0	-2	0	-2
1	1	1	2	0	1	1	1	1
1	0	1	-1	-1	0	0	-2	-2
1	-1	1	2	0	-1	1	1	1
1	-1	0	-1	1	0	-2	0	-2
1	-1	-1	2	0	1	1	1	1
1	0	-1	-1	-1	0	0	-2	-2
1	1	-1	2	0	-1	1	1	1
Eigenvalues								
λ_0^+	λ_1^-	λ_2^-	λ_1^+	λ_2^+	λ_3^+	λ_3^-	λ_4^-	λ_4^+

 $\lambda_0^+ \to 0, \lambda_1^- \to 0, \lambda_2^- \to 0, \lambda_1^+ \to \nu_{\xi}, \lambda_2^+ \to \nu, \lambda_3^+ \to \nu.$

Link-model LM, (2005)



Symmetric part: $f_{q}^{+} = \frac{1}{2}(f_{q} + f_{\bar{q}})$

Antisymmetric part: $f_{q}^{-} = \frac{1}{2}(f_{q} - f_{\bar{q}})$

– Link:
$$\{ec{c}_q,ec{c}_{ar{q}}\}$$
, $ec{c}_q=-ec{c}_{ar{q}}$

- $Collision_q = p_q + m_q$
 - $p_q = \lambda_q^+ (f_q^+ e_q^+)$ Symmetric collision part:
- Antisymmetric collision part: $m_q = \lambda_q^- (f_q^- e_q^-)$
- Local equilibrium: $e_q = e_q^+ + e_q^-$, $e_q = e_q(\mathbf{f})$

Microscopic conservation laws with Link Model

BGK:
$$\lambda^+ = \lambda^- = \lambda$$

(Qian, d'Humières &
Lallemand, 1992)
 $[\mathcal{A} \cdot (\mathbf{f} - \mathbf{e})]_q = \lambda (f_q - e_q)$

BGK⊂ TRT⊂ MRT BGK⊂ TRT⊂ LM - Conserved mass quantity $\rho(\vec{r},t)$: Let $\rho(\vec{r},t) = \sum_{q=0}^{Q-1} f_q = \sum_{q=0}^{Q-1} f_q^+ =$ $\sum_{q=0}^{Q-1} e_q = \sum_{q=0}^{Q-1} e_q^+, \text{ then } \\ \sum_{q=0}^{Q-1} \lambda_q^+ (f_q^+ - e_q^+) = 0 \text{ if } \lambda_q^+ = \lambda^+.$ - Conserved d-dimensional momentum quantity $\vec{j}(\vec{r},t)$: Let $\vec{j}(\vec{r},t) = \sum_{a=1}^{Q-1} f_q \vec{c}_q = \sum_{q=1}^{Q-1} f_q^- \vec{c}_q =$ $\sum_{q=1}^{Q-1} e_q \vec{c}_q = \sum_{q=1}^{Q-1} e_q^- \vec{c}_q$, then $\sum_{q=1}^{Q-1} \lambda_q^- (f_q^- - e_q^-) \vec{c}_q = 0 \quad \text{if} \quad \lambda_q^- = \lambda^-.$

Following idea of Chapman-Enskog (1916-1917)

- Let $\mathcal{E} = \frac{1}{L}$ with L as a characteristic length
- Let $x' = \varepsilon x$
- Let $t_1 = \varepsilon t$, $t_2 = \varepsilon^2 t$, ...
 - $\partial_t = \varepsilon \partial_{t_1} + \varepsilon^2 \partial_{t_2} + \dots$

- Population expansion around the equilibrium: $f_a = e_a + \varepsilon f_a^{[1]} + \varepsilon^2 f_a^{[2]} + \dots$
 - Collision components : $p_q^{[n]} = \left[\mathcal{A} \mathbf{f}^{[n]}\right]_q^+,$ $m_q^{[n]} = \left[\mathcal{A} \mathbf{f}^{[n]}\right]_q^-.$
 - Macroscopic laws:

$$\begin{split} & \Sigma_{q=0}^{Q-1} [p_q^{[1]} + p_q^{[2]}] = 0, \\ & \Sigma_{q=0}^{Q-1} [m_q^{[1]} + m_q^{[2]}] \vec{c}_q = 0 \end{split}$$

Directional Taylor expansion, $\partial_q = \nabla \cdot \vec{c}_q = \varepsilon \partial_{q'}$

- Evolution equation:
$$f_q(\vec{r} + \vec{c}_q, t+1) - f_q(\vec{r}, t) = \sum_n \varepsilon^n (p_q^{[n]}(\vec{r}, t) + m_q^{[n]}(\vec{r}, t)).$$

Inversion is trivial for LM : $f_q^{+[n]} = \frac{p_q^{[n]}}{\lambda^+},$ $f_q^{-[n]} = \frac{m_q^{[n]}}{\lambda_q^-}.$

- Eigenvalue functions:

$$\Lambda^{+} = -(\frac{1}{2} + \frac{1}{\lambda^{+}}) > 0,$$

$$\Lambda_{q}^{-} = -(\frac{1}{2} + \frac{1}{\lambda_{q}^{-}}) > 0.$$

- First order expansion:

$$\varepsilon p_q^{[1]} = \varepsilon (\partial_{t_1} e_q^+ + \partial_{q'} e_q^-),$$

$$\varepsilon m_q^{[1]} = \varepsilon (\partial_{t_1} e_q^- + \partial_{q'} e_q^+).$$

- Second order expansion:

$$\begin{split} & \epsilon^2 p_q^{[2]} = \epsilon^2 \partial_{t_2} e_q^+ - \epsilon (\partial_{t_1} \Lambda^+ p_q^{[1]} + \partial_{q'} \Lambda_q^- m_q^{[1]}), \\ & \epsilon^2 m_q^{[2]} = \epsilon^2 \partial_{t_2} e_q^- - \epsilon (\partial_{t_1} \Lambda_q^- m_q^{[1]} + \partial_{q'} \Lambda^+ p_q^{[1]}). \end{split}$$



Isotropic weights:

$$\Sigma_{q=1}^{Q-1} t_q^* c_{q\alpha} c_{q\beta} = \delta_{\alpha\beta},$$

$$\Sigma_{q=1}^{Q-1} t_q^* c_{q\alpha}^2 c_{q\beta}^2 = \frac{1}{3},$$

$$\alpha \neq \beta.$$

TRT + isotropic weights

$$e_q = t_q^{\star}(P(\rho) + j_q), \ j_q = \vec{j} \cdot \vec{c}_q, \ \vec{j} = \sum_{q=1}^{Q-1} t_q^{\star} j_q \vec{c}_q$$

(1) Stokes equation for pressure *P* and momentum \vec{j} : Kinematic viscosity: $v = \frac{1}{3}\Lambda^+$

(2) Isotropic linear convection-diffusion equation when $P = c_e \rho \ (0 < c_e < 1)$ and $\vec{j} = \rho \vec{U}$

Diffusion coefficients: $D_{\alpha\alpha} = c_e \Lambda^-, \forall \alpha = 1, \cdots, d$ $3 i_a^2 - |i|^2$

$$e_q = t_q^{\star}(P(\rho) + \frac{s_{j_q} + j_{j_1}}{2\rho} + j_q)$$

(1) Navier-Stokes equation (2) Isotropic linear convection-diffusion equation without second order numerical diffusion $O(\Lambda^- U_{\alpha} U_{\beta})$

"Magic parameter" $\Lambda^{\pm} = \Lambda^{+} \Lambda^{-}$ is free for both equations.

Let
$$P = c_s^2 \rho$$

Mach number: $Ma = \frac{U}{c_s}$, U is characteristic velocity.

Sound velocity: $0 < c_s^2 < 1$ **best** : $c_s^2 = \frac{1}{3}$ (Lallemand & Luo, 2000) Incompressible Navier-Stokes equation - MRT/TRT/BGK with forcing S_q^- : $f_q(\vec{r} + \vec{c}_q, t + 1) = f_q(\vec{r}, t) + p_q + m_q + S_q^-$.

Incompressible limit, $Ma \rightarrow 0$: $\rho = \rho_0(1 + Ma^2P')$, $P' = \frac{P(\rho) - P(\rho_0)}{\rho_0 U^2}$,

 $\nabla \cdot \vec{u} = O(-Ma^2 \partial_t P') = O(\varepsilon^3)$ if $U = O(\varepsilon)$

$$\rho_{0}\partial_{t}\vec{u} + \rho_{0}\nabla \cdot (\vec{u}\otimes\vec{u}) = -\nabla P + \nabla \cdot (\rho_{0}\nu\nabla\vec{u}) + \vec{F} + O(\varepsilon^{3}) + O(Ma^{2})$$

Force: $\vec{F} = \sum_{q=1}^{Q-1} S_{q}^{-}\vec{c}_{q}$
 $\vec{j} = \sum_{q=1}^{Q-1} f_{q}\vec{c}_{q} + \frac{1}{2}\vec{F}, \vec{u} = \frac{\vec{j}}{\rho_{0}}$

Kinetic boundary problem

Boundary nodes: fluid nodes with at least one outside neighbor



Dirichlet velocity condition \bullet via the bounce-back

$$f_{\bar{q}}(\vec{r}_{b}) = \tilde{f}_{q}(\vec{r}_{b}) - 2e_{q}^{-}(\vec{r}_{b} + \delta_{q}\vec{c}_{q})$$

Dirichlet pressure condition \bullet via the anti-bounce-back













No-slip condition via bounce-back reflection I. Ginzburg & P. M. Adler, J.Phys.II France, **1994**



- First order closure relation: $j_q(\vec{r}_b) + \frac{1}{2}\partial_q j_q(\vec{r}_b) = O(\epsilon^2), \ \delta_q = \frac{1}{2}$
- Second order closure relation: $j_q(\vec{r}_b) + \frac{1}{2}\partial_q j_q(\vec{r}_b) + \frac{1}{2}\frac{4}{3}\Lambda^{\pm}\partial_q^2 j_q(\vec{r}_b) = O(\epsilon^3)$
- For Poiseuille flow, effective width *H* of the channel is $H^2 = h^2 + \frac{16}{3}\Lambda^{\pm} 1$

Permeability measurements with the bounce-back reflection

- Darcy law: $\nu \vec{j} = \mathbf{K} (\vec{F} - \nabla P)$
- Permeability is viscosity dependent for BGK, $\Lambda^{\pm} = 9\nu^2$
- Permeability is absolutely viscosity independent for TRT

if
$$\Lambda^- = \Lambda^\pm / \Lambda^+$$

and Λ^{\pm} is fixed



• WHY ??

Steady recurrence equations (2006)

- Equivalent link-wise finite-difference form:

$$p_q = \lambda^+ n_q^+ = \bar{\Delta}_q e_q^- - \Lambda^- \Delta_q^2 e_q^+ + (\Lambda^\pm - \frac{1}{4}) \Delta_q^2 p_q$$

$$m_q = \lambda^- n_q^- = \bar{\Delta}_q e_q^+ - \Lambda^+ \Delta_q^2 e_q^- + (\Lambda^\pm - \frac{1}{4}) \Delta_q^2 m_q$$

- where link-wise f.d. operators are:

$$\bar{\Delta}_q \phi(\vec{r}) = \frac{1}{2} (\phi(\vec{r} + \vec{c}_q) - \phi(\vec{r} - \vec{c}_q))$$

$$\Delta_q^2 \phi(\vec{r}) = \phi(\vec{r} + \vec{c}_q) - 2\phi(\vec{r}) + \phi(\vec{r} - \vec{c}_q) , \forall \phi .$$

1

Look for solution as expansion around the equilibrium:

$$p_{q} = p_{q}(\mathbf{e}^{-}) - 2\Lambda^{-}p_{q}(\mathbf{e}^{+}) ,$$

$$m_{q} = m_{q}(\mathbf{e}^{+}) - 2\Lambda^{+}m_{q}(\mathbf{e}^{-}) ,$$

where

$$p_{q}(\mathbf{e}^{+}) = \sum_{k=1,2,...} T_{q}^{(2k)}(\mathbf{e}^{+}) ,$$

$$p_{q}(\mathbf{e}^{-}) = \sum_{k=1,2,...} T_{q}^{(2k-1)}(\mathbf{e}^{-}) ,$$

$$m_{q}(\mathbf{e}^{+}) = \sum_{k=1,2,...} T_{q}^{(2k-1)}(\mathbf{e}^{+}) ,$$

and

$$T_{q}^{(2k)}(\mathbf{e}) = \frac{a_{2k}\partial_{q}^{2k}e_{q}}{a_{k}^{2k}e_{q}}$$

$$T_q^{(2k)}(\mathbf{e}) = \frac{a_{2k}o_q c_q}{(2k)!},$$

$$T_q^{(2k-1)}(\mathbf{e}) = \frac{a_{2k-1}o_q^{(2k)}}{(2k-1)!},$$

Solution for the coefficients of the series, $k \ge 1$:

$$a_{2k-1} = 1 + +2(\Lambda^{\pm} - \frac{1}{4})\sum_{1 \le n < k} a_{2n-1} \frac{(2k-1)!}{(2n-1)!(2(k-n))!} a_{2k} = 1 + 2(\Lambda^{\pm} - \frac{1}{4})\sum_{1 \le n < k} a_{2n} \frac{(2k)!}{(2n)!(2(k-n))!}$$

- Non-dimensional steady solutions on the fixed grid

$$\vec{j'} = \frac{\vec{j}}{\rho_0 U}, P' = \frac{P - P_0}{\rho_0 U^2}$$
 are the same if
 $Ma = \frac{U}{c_s}, Fr = \frac{U^2}{gL}, Re = \frac{UL}{V}$ and Λ^{\pm} are fixed

 Provided that this property is shared by the microscopic boundary schemes,

the permeability is the same if Λ^{\pm} is fixed !!!

Multi-reflection Dirichlet boundary schemes (2003).

Boundary surface cuts at $\vec{r}_b + \delta_q \vec{c}_q$ the link between boundary node \vec{r}_b and an outside one at $\vec{r}_b + \vec{c}_q$.



Coefficients are adjusted to fit a prescribed Dirichlet value via the Taylor expansion along a link:



Linear schemes: exact for linear velocity/constant pressure.
 MR schemes: exact for parabolic velocity/linear pressure.

Stokes and Navier-Stokes flow in a square array of cylinders.

Error (in percents) of different methods in Stokes regime in 66 ² box								
ø	Edwards, FE	Bounce-back	Linear	Multi-reflection	Ghaddar, FE			
0.2	2.54	-1.63	5.5×10^{-2}	-6.5×10^{-2}	-2.4×10^{-2}			
0.3	0.53	0.78	0.51	2.8×10^{-2}	9.8×10^{-3}			
0.4	-0.64	-4.86	0.13	-9.2×10^{-2}	-2.2×10^{-2}			
0.5	-2.54	-1.1	-0.95	-8.9×10^{-3}	3.4×10^{-2}			
0.6	-8.36	-6.9	0.55	-2.1×10^{-1}	1.3×10^{-2}			

- Stokes quasi-analytical solution (Hasimoto, 1959) : $\frac{F^d}{l} = \frac{4\pi\mu\overline{U}}{k^*(\phi)}$, $k = \frac{V}{4\pi l}k^*$, ϕ is the relative solid square fraction ($\phi_{\text{max}} = \pi/4$).
- Apparent (NSE) permeability is computed from Darcy Law.
- **Dimensionless** permeability versus Re number is plotted:
 - (1) **Top picture: NSE permeability/Stokes quasi-analytical solution.**
 - (2) **Bottom picture:NSE permeability/Stokes numerical value**.







Application of multi-reflections for moving boundaries

Pressure distribution around three spheres moving in a circular tube









Solutions beyond the Chapman-Enskog expansion

$$p_{q} = p_{q}^{ch} + g_{q}^{+}, m_{q} = m_{q}^{ch} + g_{q}^{-}$$

$$g_{q}^{+} = (\Lambda^{\pm} - \frac{1}{4})\Delta_{q}^{2}g_{q}^{+}, \sum_{q=0}^{Q-1} g_{q}^{+} = 0$$

$$g_{q}^{-} = (\Lambda^{\pm} - \frac{1}{4})\Delta_{q}^{2}g_{q}^{-}, \sum_{q=1}^{Q-1} g_{q}^{-}\vec{c}_{q} = 0$$

Example of Knudsen layer in horizontal channel: e.g.,**exact Poiseuille flow using non-linear equilibrium**

$$g_q^+ = (3c_{qx}^2 - 1)t_q^*K^+(y)c_{qy}^2$$

$$g_q^- = (3c_{qx}^2 - 1)t_q^*K^-(y)c_{qy}$$

$$K^{\pm}(y) = k_1^{\pm}r_0^y + k_2^{\pm}r_0^{-y}, r_0 = \frac{2\sqrt{\Lambda^{\pm}+1}}{2\sqrt{\Lambda^{\pm}-1}}$$

$$r_0 \text{ and } 1/r_0 \text{ obey: } (r+1)^2 = 4\Lambda^{\pm}(r-1)^2$$

 $\Lambda^{\pm} = \frac{1}{4}$: accommodation in boundary node

- $h[L] = -\psi(\theta)/\rho g$ $\psi(\theta)$ capillary pressure
- $K[L T^{-1}]$ hydraulic conductivity, $K = K_r K_s$
- $K_s[L T^{-1}]$ saturated hydraulic conductivity, $K_s = k\rho g/\mu$
- $K_r(h) = k_{rw}$ dimensionless relative hydraulic conductivity
- *k*K^a permeability tensor
 K^a is dimensionless tensor
 K^a = | in isotropic case

- **Richards' equation:** $\partial_t \theta + \nabla \cdot \vec{u} = 0$, $\vec{u} = -K(h)\mathbf{K}^a \cdot (\nabla h + \vec{1}_g)$. - Conserved variable: moisture content $\theta(\vec{r}, t)$.
- Characteristic scaling: $h^{lb} = \mathcal{L}h^{phys}$, $K^{lb} = \mathcal{U}K^{phys}$.
- Coordinate scaling: $\Delta \vec{r}^{lb} = \mathcal{L} \mathbf{H} \cdot \Delta \vec{r}^{phys} = 1$, $\mathbf{H} = \text{diag}(l_x, l_y, l_z)$.
- LB grid:



Generic advection and anisotropic dispersion equation (AADE).

- LM:
$$f_q(\vec{r} + \vec{c}_q, t+1) = f_q(\vec{r}, t) + m_q + p_q + S_q^+$$

- Equilibrium: $e_q = t_q P(\rho) + t_q^* j_q$, $q = 1, \dots, Q-1$
- Immobile population: $e_0 = \rho \sum_{q=1}^{Q-1} e_q^+$ - AADE: $\partial_t \rho + \nabla \cdot \vec{j} = \nabla \cdot \vec{D} + M, M = \sum_{q=0}^{Q-1} S_q^+$
- Diffusive flux: $-\vec{D} = -\sum_{q=1}^{Q-1} \Lambda_q^- m_q \vec{c}_q$, $D_{\alpha} = \mathsf{D}_{\alpha\beta} \partial_{\beta} P(\mathbf{\rho}), \alpha = 1, \dots, d, \beta = 1, \dots, d$
- Diffusion tensor: $D_{\alpha\beta} = \sum_{q=1}^{Q-1} \mathcal{T}_q c_{q\alpha} c_{q\beta}$, $\mathcal{T}_q = \Lambda_q^- t_q$



- LM-operator has (Q-1)/2 Λ_q^- -freedoms for $\mathsf{D}_{lphaeta}$
- MRT-operator has only d eigenvalue freedoms for $D_{\alpha\alpha}$

Richards' equation via the AADE.



 $\rho = \theta, e_q = t_q P(\rho) + t_q^* j_q, \ \vec{j} = -K(\theta) \mathbf{K} \cdot \vec{1}_g.$ $\partial_t \rho + \nabla \cdot \vec{j} = \nabla \cdot k(P) \mathbf{K}^{\mathbf{a}} \nabla P(\rho).$

- Mixed form, θ/h -based
 - $P = h(\theta), k(P) = K(\theta).$
- Moisture content form, 0-based

 $P = \theta, k(P) = K(\theta) \partial_{\theta} h(\theta).$

• Kirchoff transform, θ/P -based

 $P = \int_{-\infty}^{h(\theta)} K(h') dh', \, k(P) = 1.$

VGM Sandy soil:

 $\alpha = 3.7m^{-1}, n = 5$

Original VGM (1980):

 $\partial_{\theta} h(\bar{\theta} = 1)$ is unbounded $1/\gamma = \partial_{\theta} h(1 - 10^{-6}) = 3566.24 m$

Modified VGM (T. Vogel et all, 2001): $\partial_{\theta}h(h_s) < \infty$, $h_s < 0$ Heavy rainfall episodes, Project "Dynamics of shallow water tables", http://www-rocq.inria.fr/estime/DYNAS.

physical axis parallel to LB axis.



- Compared to finite element solutions,
 E. Beaugendre et.al, 2006.
- No-flow condition except for open surface.
- Seepage face conditions on open surface.
- Explicit in time,
 Multi-reflection boundary schemes.

Reduced vertical velocity on open surface, u_z/K_s .



- Compared to finite element solutions,
 E. Beaugendre et.al, 2006.
- Rainfall intensity is $q_{in} = 0.1 K_s$ for all soils.
- FE grid with 280 nodes on the open surface.
- LB grid with 70 nodes on the open surface.

- d2Q4: 2 links for D_{xx}, D_{yy} - d3Q7: 3 links for D_{xx}, D_{yy}, D_{zz}



- **d2Q9** : **4** links for D_{xx} , D_{yy} , D_{xy}
- d3Q13 : 6 links for 6 diff. coeff.
- d3Q15 : 7 links for 6 diff. coeff.
- d3Q19 : 9 links for 6 diff. coeff.

- Solution for $\mathcal{T}_{q} = \Lambda_{q}^{-} t_{q}$, $\mathsf{D}_{\alpha\beta} = \sum_{q=1}^{Q-1} \mathcal{T}_{q} c_{q\alpha} c_{q\beta}$. - Coordinate links: $\mathcal{T}_{\alpha} = \frac{1}{2} (\mathsf{D}_{\alpha\alpha} - s_{\alpha})$, $\alpha = 1, ..., d$
- Free parameters: $s_{\alpha} = 2 \sum_{q(diag)} T_q c_{q\alpha}^2$
- Diagonal links: $d2Q9: \mathcal{T}_q = \frac{1}{4}(s_{\alpha} + \mathsf{D}_{xy}c_{qx}c_{qy}), \ s_{\alpha} = s_x = s_y$

$$\mathbf{d3Q19}: \mathcal{T}_q = \frac{1}{4}(s_{\alpha\beta} + \mathsf{D}_{\alpha\beta}c_{q\alpha}c_{q\beta}) , \ s_{\alpha\beta} = \frac{s_{\alpha} + s_{\beta} - s_{\gamma}}{2}$$

- Positivity of the equilibrium weights $t_q \ge 0$ ($\mathcal{T}_q = \Lambda_q^- t_q \ge 0$): $|\mathsf{D}_{\alpha\beta}| \le s_{\alpha\beta}, s_{\alpha} = (s_{\alpha\beta} + s_{\alpha\gamma}) \le \mathsf{D}_{\alpha\alpha}, \mathsf{D}_{\alpha\alpha} \ge 0$ may restrict the range of the off-diagonal coefficients:
- **d2Q9** : $|D_{xy}| \le \min\{D_{xx}, D_{yy}\} \Longrightarrow$ **positive definite**
- d3Q19: $|D_{\alpha\beta}| + |D_{\alpha\gamma}| \le D_{\alpha\alpha} \Longrightarrow$ positive definite

Linear (von Neumann) stability analysis (2004-)

- Periodic, linear in space solution: $\mathbf{f}(\vec{r},t) = \Omega^t K_x^x K_y^y K_z^z \mathbf{f}^*$
- Evolution equation: $(I + \mathcal{A} \cdot (I \mathcal{E})) \cdot \mathbf{f}^* = \Omega \mathcal{K} \cdot \mathbf{f}^*,$ $\mathcal{K} = \operatorname{diag}(K_x^{c_{qx}}, K_y^{c_{qy}}, K_z^{c_{qz}})$
- If $|\Omega| > 1$ for any wave-vectors (K_{χ}, K_{y}, K_{z}) the model is unstable, otherwise the model is stable: $\Omega \mathbf{f}^{*} = \mathcal{K}^{-1} \cdot (I + \mathcal{A} \cdot (I - \mathcal{E})) \cdot \mathbf{f}^{*}$
- Principal analytical result (with help of Miller's Theorems, 1971):

For advection-diffusion TRT model,

if $\Lambda^{\pm} = \Lambda^{+}\Lambda^{-} = \frac{1}{4}$, i.e. $\lambda^{+} + \lambda^{-} = -2$, then condition $\Omega^{2} = 1$ is equivalent for any Λ^{+} and Λ^{-}



- Positivity of immobile weight: $0 \le \frac{e_0}{0} \le 1$
- Minimal stencils:



 $- \forall \Delta_t$ and $\forall \Delta_x$ the model is stable if $\Lambda^{-} > \frac{\Delta_{t} \sum_{\alpha=1}^{d} D_{\alpha \alpha}}{\Delta_{x}^{2}},$ - or, $\Delta_{t} < \Lambda^{-} \frac{\Delta_{x}^{2}}{\sum_{\alpha=1}^{d} D_{\alpha \alpha}}, \Lambda^{-}$ is arbitrary.

Stability/accuracy is adjusted with Λ^+ $(\Lambda^\pm=rac{1}{4}).$

- LB with $\Lambda^+ = \Lambda^- = \frac{1}{2} \Leftrightarrow$ Forward-time central scheme (FTCS)



minimal stencils

If
$$e_q^+ \rightarrow t_q \rho(1 + \frac{3U_q^2 - |U|^2}{2})$$
, then
 $D_{\alpha\alpha} \rightarrow D_{\alpha\alpha} + \frac{U_{\alpha}^2 \Delta_t}{2}$
LB with $\Lambda^+ = \Lambda^- = \frac{1}{2} \Leftrightarrow$
MFTCS or Lax-Wendroff

Richards' equation in heterogeneous media



- First order: $[P^R \sum_{q \in I} t_q^R](\vec{r}^I) = [P^B \sum_{q \in I} t_q^B](\vec{r}^I)$ Continuity of the diffusion variable in stratified soil: $P^R(\vec{r}^I) = P^B(\vec{r}^I) + O(\epsilon^2)$ if only $\sum_{q \in I} t_q^R = \sum_{q \in I} t_q^B$
- Mixed form:

 $P^R=h^R$, $P^B=h^B$ then $h^R(\vec{r}^I)=h^B(\vec{r}^I)$

- Moisture content form: $P^R = \theta^R$, $P^B = \theta^B$ then $\theta^R(\vec{r}^I) = \theta^B(\vec{r}^I)$, $h^R(\vec{r}^I) \neq h^B(\vec{r}^I)$
- Kirchoff transform: $P(\theta) = \int_{-\infty}^{h(\theta)} K(h') dh'$

 $h^{R}(\vec{r}^{I}) \neq h^{B}(\vec{r}^{I})$ if $K^{R}(h) \neq K^{B}(h)$ or $h^{R}(\theta) \neq h^{B}(\theta)$

Drainage tube from Marinelli & Durnford (1998)

- Pressure head at the base (z = 0) is reduced from the hydrostatic to the atmospheric value
- medium-grained sand is in the middle between fine-grained sands: $K_s^{middle}/K_s^{top} = 100$
- Mixed LB formulation with $\Delta x = 1/150 m$, $\Delta t = 1/150 h$

- Minimum Δx of the adaptive implicit RK method is $\Delta x \approx 10^{-8} - 10^{-7}m$, $\Delta t = 3h$



Anisotropic weights (TRT-A) or Anisotropic eigenvalues (LM-I)

- No interface layers if only $\mathcal{T}_q^R \partial_q P^R = \mathcal{T}_q^B \partial_q P^B$, $\mathcal{T}_q = \Lambda_q^- t_q$ Vertical flow, necessary: $\mathcal{T}_q^B / \mathcal{T}_q^R = [t_q \Lambda_q^-]^B / [t_q \Lambda_q^-]^R = \mathsf{D}_{zz}^B / \mathsf{D}_{zz}^R$

if only 2.5 presure head h, [m] 1.5 2 2.5 1.5

TRT-A:
isotropic
$$\{\Lambda_q^-\} = \Lambda^-, \forall q$$

anisotropic weights $\{t_q\}$
 $P^R(\vec{r}^I) = P^B(\vec{r}^I)$ if only
 $\frac{\Lambda^{-B}}{\Lambda^{-R}} = \frac{\mathsf{D}^B_{ZZ}}{\mathsf{D}^R_{ZZ}}$

LM-I: isotropic weights:

$$t_q^R = t_q^B = c_e t_q^{\star}, \forall q$$

anisotropic $\{\Lambda_q^-\}$
Exact only if
 $\Lambda_q^{-B} = D^B$

$$\frac{\Lambda_q}{\Lambda_q^{-R}} = \frac{\mathsf{D}_{zz}}{\mathsf{D}_{zz}^R}$$

Anisotropic heterogeneous stratified 3D box following M. Bakker & K. Hemker, Adv. Water. Res. 2004

- Problem: $\nabla \cdot \mathbf{K}^R \nabla h^R = 0$, z < 0, $\nabla \cdot \mathbf{K}^B \nabla h^B = 0$, z > 0
- Interface conditions: $h^R(0^-) = h^B(0^+)$, $K^R_{zz} \partial_z h^R(0^-) = K^B_{zz} \partial_z h^B(0^+)$
- Boundary conditions: $q_x = -[K_{xx}\partial_x h + K_{xy}\partial_y h]|_{\pm X} = 0, \ \partial_y h|_{\pm Y} = -\sigma, \ q_z = -K_{zz}\partial_z h|_{\pm Z} = 0$
- From 3D to 2D: $h(x, y, z) = \phi(x, z) \sigma y + h_r$, $h_r = h(0, 0, 0)$, $\partial_x \phi^{(i)}(\pm X) = g^{(i)}, g^{(i)} = K_{xy}^{(i)} / K_{xx}^{(i)} \sigma$
- Three solutions can be distinguished for 2 layered system: Invariant along x and z: $\phi(x,z) = 0$, if $g^B = g^R = 0$ Linear along x, invariant along z: $\phi(x,z) = \frac{g^B + g^R}{2}x$, if $g^B = g^R$ Non-linear: $\phi(x,z) = (\frac{g^B + g^R}{2}x + (g^B - g^R)\phi^*(x,z))$, if $g^B \neq g^R$, $\partial_x \phi^*(\pm X, z) = \frac{1}{2} \operatorname{sign}(z)$



Anisotropic principal

xy - axis:



3D computations without interface flux corrections $K_{zz}^B/K_{zz}^R = 5$, $K_{\tau\tau}^B = K_{\tau\tau}^R$, $g^{(i)} = K_{xy}^{(i)}/K_{xx}^{(i)} = \frac{1}{8}\text{sign}(z)$

solution: $\phi(x,z) = (g^B - g^R)\phi^*(x,z), \ \partial_x\phi^*(\pm X,z) = \frac{1}{2}\text{sign}(z)$ interface links: $t_q^R \Lambda_q^{-R} \neq t_q^B \Lambda_q^{-B}, \ \Phi_{qx}^R(0^-) \neq \Phi_{qx}^B(0^+)$



Leading order interface corrections

- **Piece-wise linear solution for** i^{th} layer: $f_q^{(i)} = [e_q + t_q \partial_q P(x, y, z) / \lambda_q^-]^{(i)}, P^R(\vec{r}^I) = P^B(\vec{r}^I)$ Then $\partial_{\tau} P^R(\vec{r}^I) = \partial_{\tau} P^B(\vec{r}^I)$, and $D^R_{zz} \partial_z P^R(\vec{r}^I) = D^B_{zz} \partial_z P^B(\vec{r}^I)$
- No interface layers if each flux component is continuous: $\Phi_{q\alpha}^{R} = \Phi_{q\alpha}^{B}$, i.e. $t_{q}^{R}\Lambda_{q}^{-R}\partial_{\alpha}P^{R}c_{q\alpha} = t_{q}^{B}\Lambda_{q}^{-B}\partial_{\alpha}P^{B}c_{q\alpha}$, $\forall q \in I$
- Piece-wise linear solutions for any anisotropy and heterogeneity via the interface corrections

$$f_{q}(\vec{r}^{B}, t+1) = \tilde{f}_{q}^{R}(\vec{r}^{R}, t) + (\delta_{q}^{+R} + \delta_{q}^{-R}),$$

$$f_{\bar{q}}(\vec{r}^{R}, t+1) = \tilde{f}_{\bar{q}}^{B}(\vec{r}^{B}, t) + (\delta_{\bar{q}}^{+B} + \delta_{\bar{q}}^{-B})$$

Diffusion variable: $\delta_{q}^{+R} = S_{q}^{R}(r_{E}^{R}-1), S_{q}^{R} = e_{q}^{+R} + \frac{1}{2}m_{q}^{R} \approx e_{q}^{+R}(\vec{r}^{I})$

Fluxes: $\delta_q^{-R} = \sum_{\alpha = \{x, y, z\}} \delta_q^{-R}, \ \delta_q^{-R} = \Phi_{q\alpha}^R (r_E^R r_\Lambda^R r_\alpha^R - 1)$ with ratios: $r_E^R = t_q^B / t_q^R, \ r_\Lambda^R = \Lambda_q^{-B} / \Lambda_q^{-R}, \ r_\alpha^R = [\partial_\alpha P^B / \partial_\alpha P^R](\vec{r}^I)$

LM-I-model with interface corrections Comparison with exact and "multi-layer" solutions for $\partial_x \phi^{\star B}(x, 0^+)$ and $\partial_x \phi^{\star R}(x, 0^-)$, $K_{xy}^{(i)} = [K_{xx}^{(i)} \operatorname{sign}(z)]/2$



- Prescribed normal derivative: $\delta_n = -2\mathcal{T}_q \partial_n P(\vec{r}_{\mathrm{w}}, t) C_{an}$
- **Relaxed tangential** derivatives:

 $\delta_{\tau} = -2\mathcal{T}_q \sum_{\tau} \partial_{\tau} P(\vec{r}_{\rm b}, t) C_{q\tau},$ $\partial_{\tau} P$ is derived from the current population solution





Steady-state unconfined flow

computed with h-formulation on anisotropic grids

- Reference solution: Clement et al, J.Hydrol., 181, 1996
- Boundary conditions:

Top/bottom: No-flow via bounce-back reflection $f_{\bar{q}}(\vec{r}_{\rm b}, t+1) = \tilde{f}_q(\vec{r}_{\rm b}, t)$

West: Hydrostatic, $h^{b}(z) + z = 1 m$ via anti-bounce-back reflection $f_{\bar{q}}(\vec{r}_{b}, t+1) =$ $-\tilde{f}_{q}(\vec{r}_{b}, t) + 2t_{q}h^{b}(z)$

East: Seepage above z = 0.2 m

Uniform refining in $100^2 = 1^2 m^2$ box



Anisotropic non-uniform refining

 $l_z^{bottom} = 0.5, \ l_z^{top} = 4, \ A = l_z^{top} / l_z^{bottom} = 8$



AADE: interface collision operator (2005)

- Prescribed continuity conditions:

Diffusion variable: $e_q^{+R}(\vec{r}^I) = e_q^{+B}(\vec{r}^I) + O(\epsilon^2)$

Advective-diffusive flux components:

$$e_q^{-R} - \Lambda_q^{-R} m_q^R = e_q^{-B} - \Lambda_q^{-B} m_q^B$$

Interface collision components:

(1)
$$e_q^{-I} = \frac{1}{2}(e_q^{-R} + e_q^{-B})$$

Harmonic means:

LM-I :
$$\Lambda_q^{-I} = \frac{2\Lambda_q^{-B}\Lambda_q^{-R}}{\Lambda_q^{-B} + \Lambda_q^{-R}}$$
 if $\Lambda_q^{-R} / \Lambda_q^{-B} = m_q^B / m_q^R$
TRT-A: $\Lambda^{-I} = \frac{2\Lambda^{-B}\Lambda^{-R}}{\Lambda^{-B} + \Lambda^{-R}}$ if $\Lambda^{-R} / \Lambda^{-B} = \sum_{q \in I} m_q^B / \sum_{q \in I} m_q^R$

(2)
$$p_q^I = \frac{1}{2}(p_q^R + p_q^B)$$

- (3) Mass source: $Q_q^{+I} = \frac{1}{2}(Q_q^{+R} + Q_q^{+B})$
- (4) **Deficiency:** $P^{I} = \frac{1}{2}(P^{(R)} + P^{(B)}) + \Delta P, \Delta P = \frac{1}{4}(\partial_{z}P^{(B)} \partial_{z}P^{(R)})$



h(z)/h(0)

-0,8 -0,6 -0,4 -0,2 0 0,2 0,4 0,6 0,8 Channel width, m

12

10

8

6

4

2

0

Harmonic mean

LB Method:

- Kinetic schemes
- Finite volume and finite-difference LB
- Adaptive grids
- Thermal (hybrid) schemes
- Comparative studies of LBE, FE and FV
 - Difficult problems:
- Stabilization for high Reynolds numbers
- Stabilization for high density ratios
- Stability of boundary schemes.

Topics of International Conference for Mesoscopic Methods in Engineering and Science (ICMMES), www.icmmes.org

Applications:

- Porous media: flow+dispersion, capillary functions, relative permeabilities, acoustic properties,...
- Direct Numerical Simulations including Large-Eddy
 Simulations (LES), e.g. for external aerodynamics of a car
- Rheology for complex fluids:
 - (1) particulate suspensions
 - (2) foaming process
 - (3) multi-phase and multi-component fluids
 - (4) non-Newtonian and bio-fluids
- Flow-structure interactions and Micro-fluidics (non-continuum effects)
- Parallel, physically based animations of fluids.

References

- H. Hasimoto, On the periodic fundamental solutions of the Stokes equations and their application to viscous flow past a cubic array of spheres, J. Fluid. Mech. 5, 317, 1959.
- J. J. H. Miller, On the location of zeros of certaines classes of polynomials with application to numerical analysis, J. Inst. Maths Applics 8, 397, 1971.
- A. S. Sangani and A. Acrivos, Slow flow past periodic arrays of cylinders with application to heat transfer, Int. J.
 Multiphase Flow 8, No 3, 193, 1982.
- Hindmarsch, A.C., Grescho P.M., and Griffiths, D.F., The stability of explicit time-integration for certain finite difference approximation of the multi-dimensional advection-diffusion equation, Int.J.for Numerical Methods in Fluids. 4, 853, 1984.
- D. A. Edwards, M. Shapiro,
 P.Bar-Yoseph, and M. Shapira, The influence of Reynolds number upon the apparent permeability of spatially periodic arrays of cylinders, Phys.
 Fluids A 2 (1), 45, 1990.

- Y. Qian, D. d'Humières and P. Lallemand, Lattice BGK models for Navier-Stokes equation, Europhys. Lett. 17, 479, 1992.
- C. Ghaddar, On the permeability of unidirectional fibrous media: A parallel computational approach, Phys. Fluids 7 (11), 2563, 1995.
- P. Lallemand and L.-S. Luo, Theory of the lattice Boltzmann method: Dispersion, dissipation, isotropy, Galilean invariance, and stability.,
 Phys. Rev. E, 61, 6546, 2000.
- **I. Ginzburg and D. d'Humières**, Multi-reflection boundary conditions for lattice Boltzmann models, **Phys. Rev. E**, **68**,066614, **2003**.
- **M. Bakker and K. Hemker**, Analytic solutions for groundwater whirls in box-shaped, layered anisotropic aquifers, **Adv Water Resour**, **27**:1075, **2004**.
- Beaugendre H., A. Ern, T. Esclaffer, E. Gaume., Ginzburg I., Kao C., A seepage face model for the interaction of shallow water-tables with ground surface: Application of the obstacle-type method. Journal of Hydrology, 329, 1/2:258, 2006.
- **I. Ginzburg**, Variably saturated flow described with the anisotropic Lattice Boltzmann methods, **J. Computers and Fluids**,**35(8/9)**, 831, **2006**.
- **C. Pan, L. Luo, and C. T. Miller.** An evaluation of lattice Boltzmann schemes for porous media simulations. **J. Computer and Fluids, 35(8/9)**, 898, **2006**.