Consistent two-relaxation-times LBE model for porous flow and transport

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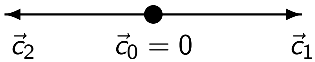
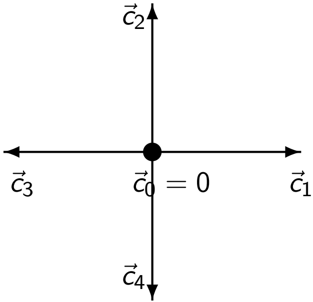
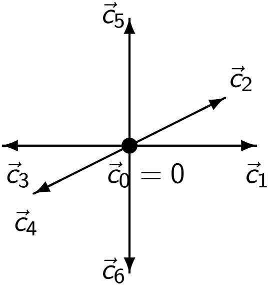
Outline

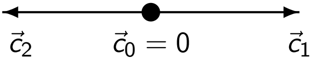
Minimal velocity sets: D1Q3, D2Q5 & D3Q7

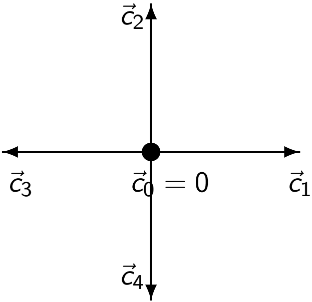


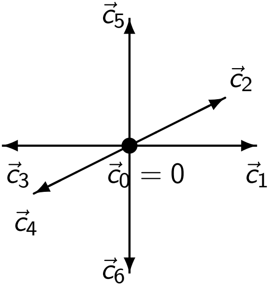




D1Q3, D2Q5 & D3Q7: anisotropic diagonal tensors

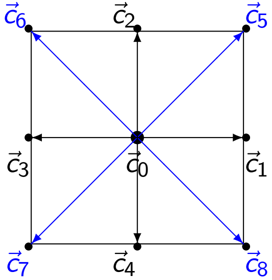




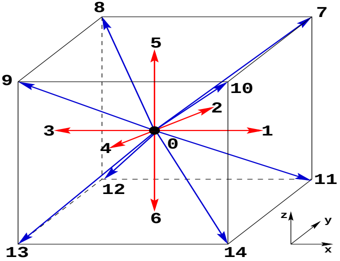


Hydrodynamic & anisotropic diffusion equations

D2Q9 but also D3Q13, D3Q19, D3Q27, ...

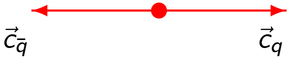


D3Q15



LINK: $\vec{c}_{\bar{q}} = -\vec{c}_q$

All elements are decomposed into their symmetric and anti-symmetric components for any pair of opposite velocities



$$
\begin{aligned}
f_q^{\pm} &= \frac{1}{2}(f_q \pm f_{\bar{q}}) \ , \ f_q = f_q^+ + f_q^- \\
e_q^{\pm} &= \frac{1}{2}(e_q \pm e_{\bar{q}}) \ , \ e_q = e_q^+ + e_q^-
\end{aligned}
$$

TRT: two-relaxation-times model (2004−)

$$f_q(\vec{r}+\vec{c}_q, t+1) = (f_q+g_q^{+}+g_q^{-})(\vec{r}, t)\ ,\ g_q^{\pm} = \lambda^{\pm} n_q^{\pm}\ ,\ n_q^{\pm} = f_q^{\pm} - e_q^{\pm}$$

Mass: $e_0 = \rho - \sum_{q=1}^{Q-1} e_q^{+}\ ,\ \rho = \sum_{q=0}^{Q-1} f_q = \sum_{q=0}^{Q-1} e_q^{+}$

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Mass: $e_0 = \rho - \sum_{q=1}^{Q-1} e_q^+\ ,\ \rho = \sum_{q=0}^{Q-1} f_q = \sum_{q=0}^{Q-1} e_q^+$

Mass source:

$$e_q^+ \Longrightarrow e_q^+ - \frac{M_q}{\lambda^+} \rightarrow \sum_{q=0}^{Q-1} g_q^+ = \sum_{q=0}^{Q-1} M_q = M\ ,$$

Momentum source:

$$e_q^- \Longrightarrow e_q^- - \frac{F_q}{\lambda^-} \rightarrow \sum_{q=0}^{Q-1} g_q^- \vec{c}_q = \sum_{q=1}^{Q-1} F_q \vec{c}_q = \vec{F}$$

TRT: two-relaxation-times model (2004−)

$$f_q(\vec{r}+\vec{c}_q, t+1) = (f_q+g_q^{+}+g_q^{-})(\vec{r}, t)\ ,\ g_q^{\pm} = \lambda^{\pm} n_q^{\pm}\ ,\ n_q^{\pm} = f_q^{\pm} - e_q^{\pm}$$

Stokes Eq. for $P(\rho)$ & $\vec{j} = \rho \vec{U}$

$$e_q^{+} = t_q^{(m)} P(\rho)\ , \quad P = c_e \rho$$

$$e_q^{-} = t_q^{(a)} (\vec{j} \cdot \vec{c}_q)\ ,\ \vec{j} = \sum_{q=1}^{Q-1} f_q \vec{c}_q$$

AADE: $\partial_t \rho + \nabla \cdot \rho \vec{U} = \nabla \cdot \mathbf{D} \nabla P$

$$e_q^{+} = t_q^{(m)} P(\rho)\ , \quad \forall\ P(\rho)$$

$$e_q^{-} = t_q^{(a)} (\vec{U} \cdot \vec{c}_q) \rho\ ,\ \forall\ \vec{U}(\rho)$$

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Stokes Eq. for $P(\rho)$ & $\vec{j} = \rho \vec{U}$

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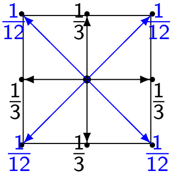
TRT: two-relaxation-times model (2004−)

Isotropic and hydrodynamic weights: $t_q^{(a)} = t_q^{(m)} = t_q^\star$

$$\sum_{q=1}^{Q-1} t_q^\star c_{q\alpha} c_{q\beta} = \delta_{\alpha\beta} \ , \ \forall \alpha, \beta \ , \ 3 \sum_{q=1}^{Q-1} t_q^\star c_{q\alpha}^2 c_{q\beta}^2 = 1 \ , \ \forall \alpha \neq \beta$$



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$$e_q^+ \Longrightarrow e_q^+ + 3 t_q^\star \rho \frac{(\vec{U} \cdot \vec{c}_q)^2 - ||\vec{U}||^2}{2}$$

Stokes $\Longrightarrow$ Navier-Stokes **D $\Longrightarrow$ D−D^{num}**

TRT: two-relaxation-times model (2004−)

Isotropic and hydrodynamic weights: $t_q^{(a)} = t_q^{(m)} = t_q^\star$

$$\sum_{q=1}^{Q-1} t_q^\star c_{q\alpha} c_{q\beta} = \delta_{\alpha\beta} \ , \ \forall \alpha, \beta \ , \ 3 \sum_{q=1}^{Q-1} t_q^\star c_{q\alpha}^2 c_{q\beta}^2 = 1 \ , \ \forall \alpha \neq \beta$$

<u>ANTI-DIFFUSION</u>+<u>NUMERICAL DIFFUSION</u>= O

$$\mathbf{D}^{eff} = \Lambda^- \begin{pmatrix} \mathcal{D}_{xx} + U_x^2 - U_x^2 & \mathcal{D}_{xy} + U_x U_y - U_x U_y \\ \mathcal{D}_{xy} + U_x U_y - U_x U_y & \mathcal{D}_{yy} + U_y^2 - U_y^2 \end{pmatrix}$$

TRT: two-relaxation-times model (2004–)

Stokes or Navier-Stokes Eqs.

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

$$\nu = \frac{\Lambda^+}{3}\ , \ \ \nu_\xi = (\frac{2}{3} - c_e)\Lambda^+$$

Isotropic linear ADE

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

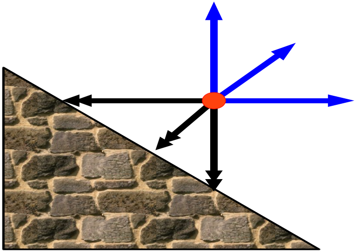
$$D_{\alpha\alpha} = \Lambda^- c_e,\ P = c_e \rho$$

"Magic" (ghost, kinetic) parameter is free:

$$\Lambda = \Lambda^- \Lambda^+ > 0$$

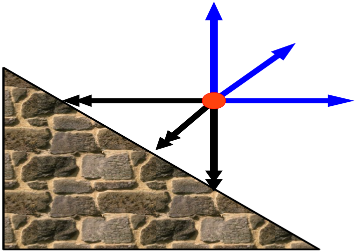
No-slip (zero velocity) condition with bounce-back:

$$f_{\bar{q}}(\vec{r}_{\mathrm{b}}, t+1) = (f_q + g_q^+ + g_q^-)(\vec{r}_{\mathrm{b}}, t)$$



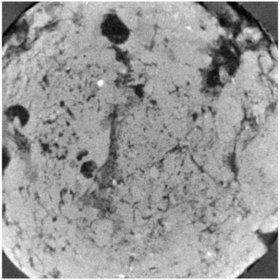
Zero concentration condition with anti-bounce-back:

$$f_{\bar{q}}(\vec{r}_{\mathrm{b}}, t+1) = -(f_q + g_q^+ + g_q^-)(\vec{r}_{\mathrm{b}}, t)$$



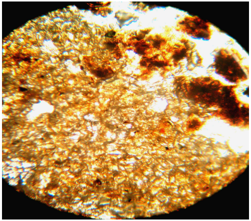
Pesticide transport in cultivated soil porosity

Valérie Pot, Nadia Elyeznasni & Hassan Hammou, l'INRA

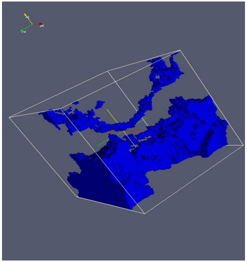


3D CT, $\approx 5\ cm$

Optical microscopy



$\approx 1mm$



Soil porosity

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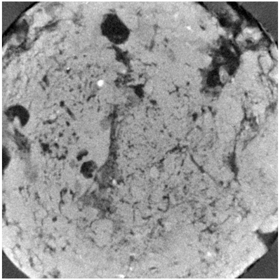

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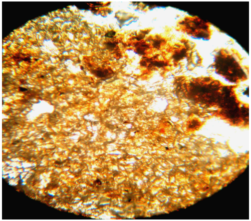
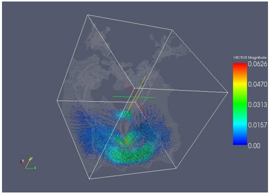


$\approx 1mm$



Stokes flow

Pesticide transport in cultivated soil porosity

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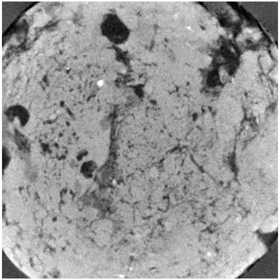

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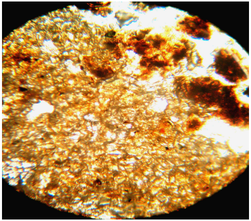
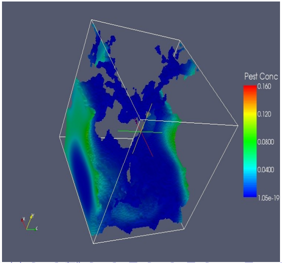


$\approx 1mm$

Pesticide plume



Pesticide transport in cultivated soil porosity

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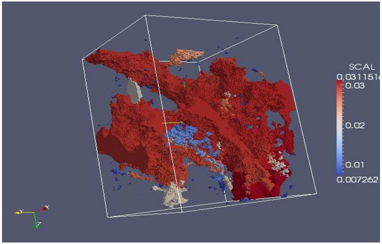
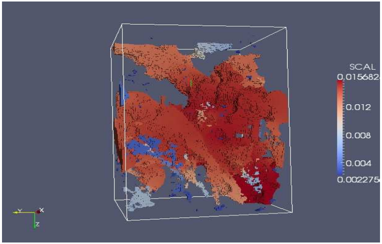


Uniform sorption

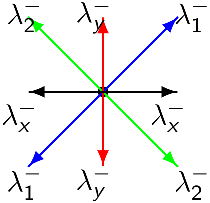


+biofilm degradation

Full anisotropic 2D and 3D diffusion tensors

ANISOTROPIC COLLISION: **L (link) -operator**

$$g_q^+(\vec{r}, t) = \lambda^+ n_q^+(\vec{r}, t)\ ,\ g_q^-(\vec{r}, t) = \lambda_q^- n_q^-(\vec{r}, t)$$

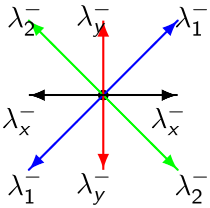


$$\Lambda^- \begin{pmatrix} 2t^{(m)}\lambda_x^- + (\frac{1}{2} - t^{(m)})(\lambda_1^- + \lambda_2^-) & (\frac{1}{2} - t^{(m)})(\lambda_1^- - \lambda_2^-) \\ D_{xy} & D_{yy} \end{pmatrix}$$

Full anisotropic 2D and 3D diffusion tensors

ANISOTROPIC COLLISION: **L (link) -operator**

$$g_q^+(\vec{r},t) = \lambda^+ n_q^+(\vec{r},t)\ ,\ g_q^-(\vec{r},t) = \lambda_q^- n_q^-(\vec{r},t)$$



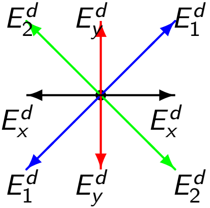
L-operator reduces to TRT for hydrodynamics: $\lambda_q^- \Longrightarrow \lambda^-$

$$\text{TRT} = \text{MRT} \cup \text{L}$$

Full anisotropic 2D and 3D diffusion tensors

Anisotropic Equilibrium:

$$e_q^+ = t_q^{(m)} P(\rho) \rightarrow E_q^+ P(\rho)$$



Full anisotropic 2D and 3D diffusion tensors

Anisotropic Equilibrium:

Diagonal links : $e_q^+ = t_q^{(m)} P(\rho) \rightarrow E_q^+ P(\rho)$

d2Q9, d3Q15 : $E_q^+ = t_q^{(m)} c_e + \frac{\sum_{\alpha \neq \beta} \mathcal{D}_{\alpha\beta} c_{q\alpha} c_{q\beta}}{\sum_{\alpha \neq \beta} c_{q\alpha} c_{q\beta}}, \; \mathcal{D}_{\alpha\beta} = \frac{D_{\alpha\beta}}{\Lambda^-}.$

Full anisotropic 2D and 3D diffusion tensors

Anisotropic Equilibrium:

Diagonal links : $e_q^+ = t_q^{(m)} P(\rho) \to E_q^+ P(\rho)$

d2Q9, d3Q15 : $E_q^+ = t_q^{(m)} c_e + \frac{\sum_{\alpha\neq\beta} \mathcal{D}_{\alpha\beta} c_{q\alpha} c_{q\beta}}{\sum_{\alpha\neq\beta} c_{q\alpha} c_{q\beta}}, \; \mathcal{D}_{\alpha\beta} = \frac{D_{\alpha\beta}}{\Lambda^-}$

Coordinate links :

Minimal models & d2Q9, d3Q15

$$E_q^+ = t_q^{(m)} c_e + \frac{1}{2} \sum_{\alpha} (\mathcal{D}_{\alpha\alpha} - c_e) c_{q\alpha}^2$$

Mean : $c_e = \frac{\sum_\alpha \mathcal{D}_{\alpha\alpha}}{d}$

Full anisotropic 2D and 3D diffusion tensors

AADE: $\partial_t \rho + \nabla \cdot \rho \vec{U} = \nabla \cdot \mathbf{D} \nabla P$

$$\begin{cases} D_{\alpha\beta} = \sum_{q=1}^{Q-1} \Lambda_q^- E_q^+ c_{q\alpha} c_{q\beta} \\ e_q^+ = E_q^+ P(\rho) \end{cases}$$

Local diffusive flux:

$$\vec{D}(\rho) = (\Lambda_q^- g_q^- \cdot \vec{c}_q) \approx D_{\alpha\beta} \nabla_\beta P(\rho)$$

Full anisotropic 2D and 3D diffusion tensors

AADE: $\partial_t \rho + \nabla \cdot \rho \vec{U} = \nabla \cdot \mathbf{D} \nabla P$

$$\begin{cases} D_{\alpha\beta} = \sum_{q=1}^{Q-1} \Lambda_q^- E_q^+ c_{q\alpha} c_{q\beta} \\ e_q^+ = E_q^+ P(\rho) \end{cases}$$

L-model

- Anisotropic $\{\Lambda_q^-\}$
- Isotropic or Anisotropic $\{E_q^+\}$

TRT-model

- Isotropic $\{\Lambda_q^- = \Lambda^-\}$
- Anisotropic $\{E_q^+\}$

TRT freedoms : full models: $\{t_q^{(m)}, t_q^{(a)}\}$

all models: $\vec{U}$, $c_e \Lambda^- = \frac{|U|}{Peclet}$, $P = c_e \rho$, and Λ

Full anisotropic 2D and 3D diffusion tensors

L-model

- Anisotropic $\{\Lambda_q^-\}$
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TRT-model

- Isotropic $\{\Lambda_q^- = \Lambda^-\}$
- Anisotropic $\{E_q^+\}$

*available anisotropy for pure diffusion

$\{E_q^+ > 0\} \Leftrightarrow |\mathcal{D}_{\alpha\beta}| \leq \min_\alpha \mathcal{D}_{\alpha\alpha}$, for d2Q9 and d3Q15.

Full anisotropic 2D and 3D diffusion tensors

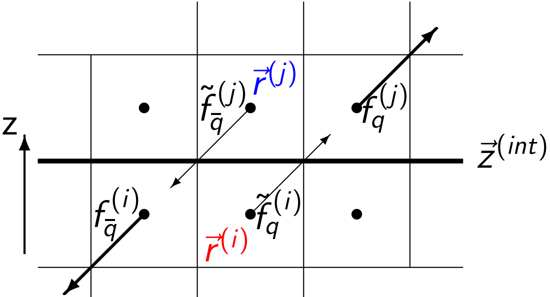
L-model

- Anisotropic $\{\Lambda_q^-\}$
- Isotropic or Anisotropic $\{E_q^+\}$

TRT-model

- Isotropic $\{\Lambda_q^- = \Lambda^-\}$
- Anisotropic $\{E_q^+\}$

Heterogeneous $\mathcal{D}_{\alpha\beta}$: discontinuous Λ_q^- or E_q^+ ?



Full anisotropic 2D and 3D diffusion tensors

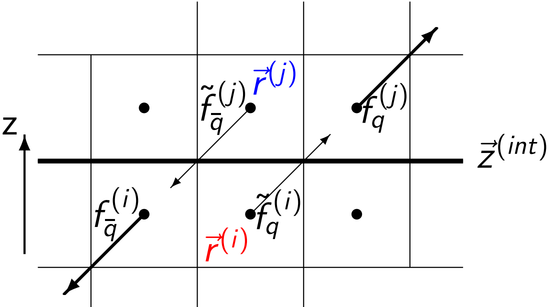
L-model

- Anisotropic $\{\Lambda_q^-\}$
- Isotropic or Anisotropic $\{E_q^+\}$

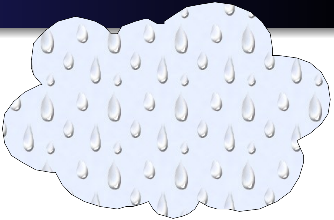
TRT-model

- Isotropic $\{\Lambda_q^- = \Lambda^-\}$
- Anisotropic $\{E_q^+\}$

Heterogeneous $\mathcal{D}_{\alpha\beta}$: discontinuous Λ_q^- or E_q^+ ? Eigenvalues Λ_q^- !

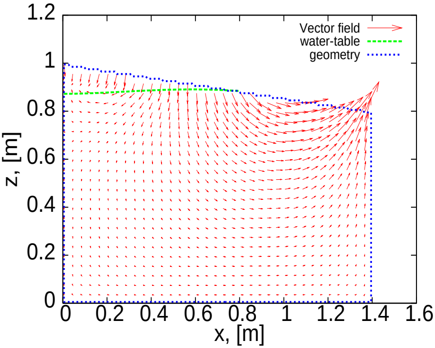


Dynamics of underground water tables under rainfall episodes



Dynas Project: l'ENPC/Cemagref/l'INRIA

2003-2004



Richard's equation for variably saturated flow

UNSATURATED ZONE: $\theta_r \leq \theta \leq \theta_s$

$$\begin{cases} \partial_t \theta + \nabla \cdot \vec{u} = 0 \\ \vec{u} = -K(\theta)\mathbf{K}^a(\nabla h(\theta) + \vec{1}_z) \end{cases}$$

SATURATED ZONE: $\theta \equiv \theta_s$

$$\begin{cases} \nabla \cdot \vec{u} = 0 \\ \vec{u} = -K_s\mathbf{K}^a(\nabla h + \vec{1}_z) \end{cases}$$

Variables

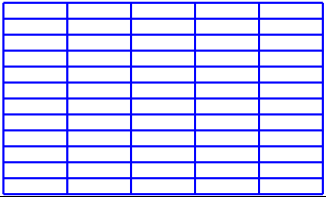
- $\theta(\vec{r}, t)$ water content
- $h(\theta)$ pressure head, $[L]$
- $K(\theta) = K_r(\theta)K_s$ hydraulic conductivity, $[L\ T^{-1}]$
- $K_r(\theta)$ relative hydraulic conductivity
- $K_s = \frac{k\rho g}{\mu}$ saturated hydraulic conductivity, $[L\ T^{-1}]$
- $k\mathbf{K}^a$ permeability tensor, $\mathbf{K}^a = \mathbf{I}$ if isotropic

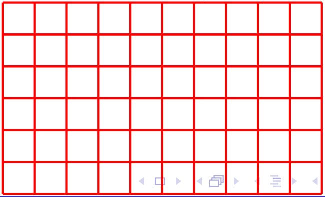
Richard's equation as the AADE

$$\partial_t \rho + \nabla \cdot \vec{j}(\rho) = \nabla \cdot \vec{D}(\rho)$$

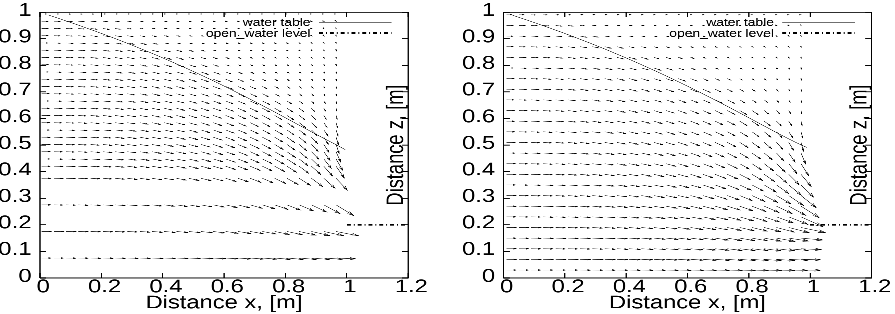
- $\rho = \theta$ — conserved quantity
- $\vec{j} = -K(\rho)[\mathbf{K^a L}\ ] \cdot \vec{1}_z$ — non-linear convective flux
- $-\vec{D} = -K(\rho)[\mathbf{L K^a L}] \cdot \nabla h(\rho)$ — non-linear diffusive flux
- $\mathbf{L} = \mathrm{diag}(l_x, l_y, l_z)$ — grid transformation

from physical *to* *cuboid (LBE) grid*





Computations on cuboid grid via anisotropic sub-grid transformations



Equilibrium forms of Richard's equation

EQUILIBRIUM: $e_q^+ = t_q^{(m)} P(\theta)$, $e_0 = \theta - \sum_{q=1}^{Q-1} e_q^+$

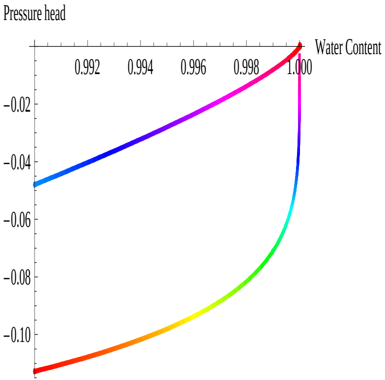
DIFFUSIVE FLUX: $\vec{D} = \Lambda^- \nabla P(\theta)$ *should fit* $\vec{D} = K(\theta) \nabla h(\theta)$

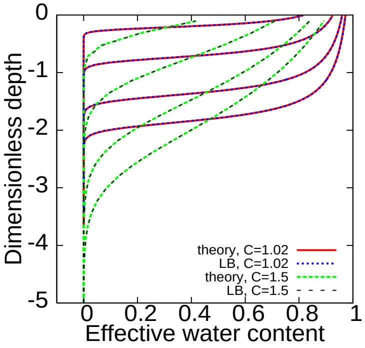
θ-based

$$P(\theta) = c_e \theta$$

$$c_e \Lambda^- = K(\theta) \partial_\theta h(\theta)$$

Equilibrium forms of Richard's equation





Equilibrium forms of Richard's equation

EQUILIBRIUM: $e_q^+ = t_q^{(m)} P(\theta)\ ,\ e_0 = \theta - \sum_{q=1}^{Q-1} e_q^+$

DIFFUSIVE FLUX: $\vec{D} = \Lambda^- \nabla P(\theta)$ *should fit* $\vec{D} = K(\theta)\nabla h(\theta)$

θ-based

$P(\theta) = c_e\theta$

$c_e\Lambda^- = K(\theta)\partial_\theta h(\theta)$

Integral transforms

$P(\theta) = c_e \int_{-\infty}^{h(\theta)} K(h')dh'$

$c_e\Lambda^- = 1$

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θ/h-based

$P(\theta) = c_e h(\theta)$

$c_e \Lambda^- = K(\theta)$

Integral transforms

$P(\theta) = c_e \int_{-\infty}^{h(\theta)} K(h')dh'$

$c_e \Lambda^- = 1$

Equilibrium forms of Richard's equation

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$c_e \Lambda^- = K(\theta)$

Integral transforms

$P(\theta) = c_e \int_{-\infty}^{h(\theta)} K(h')dh'$

$c_e \Lambda^- = 1$

Heterogeneous soils/grids: only $P(\theta) = c_e h(\theta)$ is suitable

Equilibrium forms of Richard's equation

EQUILIBRIUM: $e_q^+ = t_q^{(m)} P(\theta)\ ,\ e_0 = \theta - \sum_{q=1}^{Q-1} e_q^+$

DIFFUSIVE FLUX: $\vec{D} = \Lambda^- \nabla P(\theta)$ *should fit* $\vec{D} = K(\theta)\nabla h(\theta)$

θ-based	**θ/h-based**	**Integral transforms**
$P(\theta) = c_e\theta$	$P(\theta) = c_e h(\theta)$	$P(\theta) = c_e \int_{-\infty}^{h(\theta)} K(h')dh'$
$c_e\Lambda^- = K(\theta)\partial_\theta h(\theta)$	$c_e\Lambda^- = K(\theta)$	$c_e\Lambda^- = 1$

Non-linear equilibrium or non-linear eigenvalues ?

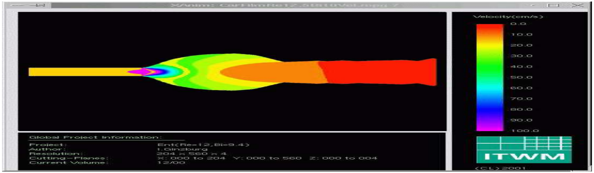
Linear stability	Non-linear stability	Improve stability ?
Stiff $\Lambda^-(\theta)$	Smoother $\Lambda^-(\theta)$	Improve sharpness ?

Filling of expanded cavity with Bingham (plastic) fluid

predictions: *A. N. Alexandrou, E. Duc & V. Entov*, 2001

$$||\mathbf{D}|| = 0 \quad \text{if} \quad ||\mathbf{T}|| < T_0 \;\; \& \;\; \mathbf{T} = (\nu + \frac{T_0}{||\mathbf{D}||})\mathbf{D} \quad \text{if} \quad ||\mathbf{T}|| > T_0$$

Reynolds$= \frac{UL}{\nu} = \mathbf{12.5}$ & **Bingham**$= \frac{T_0 L}{\nu U} = \mathbf{9.4}$

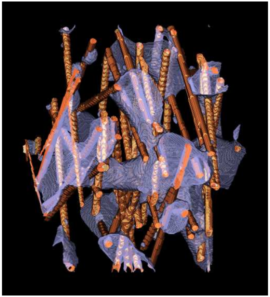


Oil distribution in anisotropic fibrous material

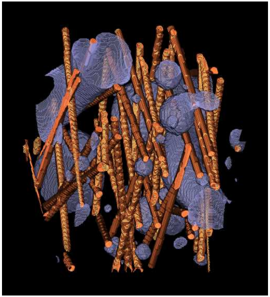
relative permeability and capillary pressure versus saturation

ITWM, 1999-2002

Fleece



Oil is wetting

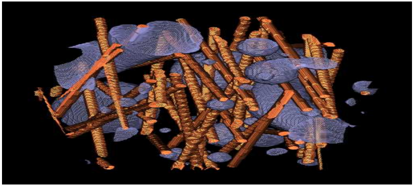


Oil is non-wetting

From mixture to steady distribution

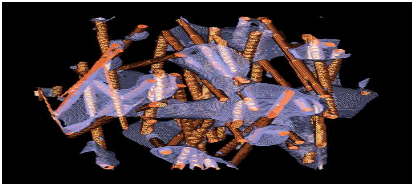
Stokes flow with $(\frac{\rho^R}{\rho^B})^{lb} = 1$ &

$(\frac{\nu^R}{\nu^B})^{lb} = (\frac{\mu^R}{\mu^B})^{phys} = (\frac{\nu^R}{\nu^B})^{phys}(\frac{\rho^R}{\rho^B})^{phys}$



From mixture to steady distribution

High viscosity values accelerate the convergence to steady state



Single-relaxation-time BGK operator*

Most popular and poor, BGK $\in$ TRT $\in$ MRT:

$$f_q(\vec{r} + \vec{c}_q, t+1) = f_q(\vec{r}, t) + \lambda(f_q - e_q) \ , \ \lambda^+ = \lambda^- = \lambda$$

*Y. Qian, D. d'Humières and P. Lallemand, *Europhys. Lett.* 1992.

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BGK = TRT in cost but BGK cannot set Magic parameter Λ

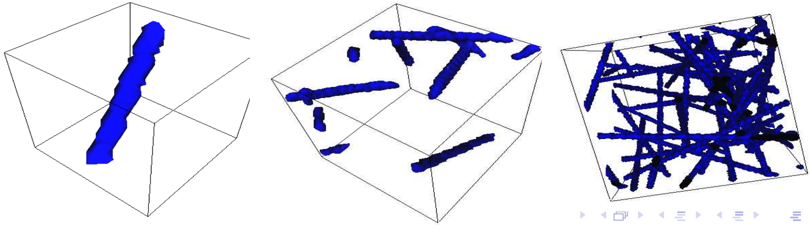
- $\Lambda = \Lambda^{-2} = \Lambda^{+2} = 9\nu^2$
- $\Lambda \to \infty$ when $\nu \to \infty$
- $\Lambda \to 0$ when $\nu \to 0$

*Y. Qian, D. d'Humières and P. Lallemand, *Europhys. Lett.* 1992.

Permeability measurements

Let us compute Stokes flow using the bounce-back,
then compute mean velocity $\bar{\vec{j}}$ and derive permeability $\mathbf{K}$ of porous structure from

$$\underline{\textbf{Darcy's Law}}: \qquad \nu\bar{\vec{j}} = \mathbf{K}\overline{(\vec{F} - \nabla P)}$$



Linear Stokes flow ?

TABLE SHOWS: $\frac{k(\Lambda^+)-k(\Lambda^+=\frac{1}{2})}{k(\Lambda^+=\frac{1}{2})}$ versus $\Lambda^+ = 3\nu$

Λ^+	20^3, $\phi \approx 0.965$		90^3, $\phi \approx 0.941$	
		BGK		**BGK**
1/8		-0.077		-0.083
15/2		4.699		2.236

- The permeability depends on the viscosity of the modeled flow when all eigenvalues are equal !

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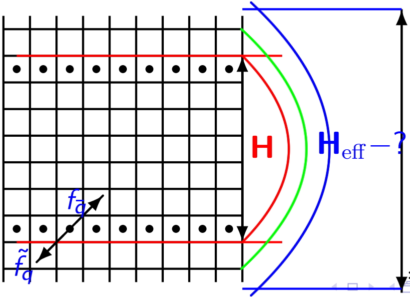
Λ^+	20^3, $\phi \approx 0.965$		90^3, $\phi \approx 0.941$	
	TRT	**BGK**	**TRT**	**BGK**
$1/8$	10^{-13}	-0.077	10^{-13}	-0.083
$15/2$	-2.8×10^{-12}	4.699	-10^{-13}	2.236

- The permeability depends on the viscosity of the modeled flow when all eigenvalues are equal !
- But it is constant when Λ is fixed (1995) !

Effective location of no-slip walls

EXACT SOLUTION*:

$$H_{\text{eff}}^2 = H^2 + \frac{16}{3}\Lambda - 1$$
$$H_{\text{eff}} = H \text{ if } \Lambda = \frac{3}{16}$$
$$H_{\text{eff}} < H \text{ if } \Lambda < \frac{3}{16}$$
$$H_{\text{eff}} > H \text{ if } \Lambda > \frac{3}{16}$$



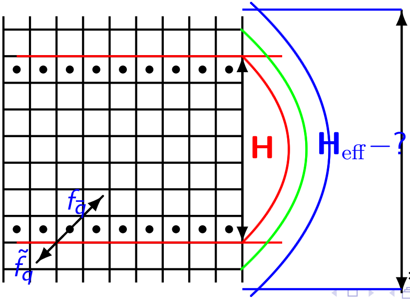
*IG & P. Adler, 1994

Effective location of no-slip walls

Bounce back permeability error:

$$\text{BGK} \quad : \quad \frac{k - k^{th}}{k^{th}} = (48\nu^2 - 1)$$

$$\text{TRT} \quad : \quad \frac{k - k^{th}}{k^{th}} = \frac{(\frac{16}{3}\Lambda - 1)}{H^2} \, .$$



*IG & P. Adler, 1994

Effective location of no-slip walls

SECOND ORDER NON-EQUILIBRIUM EXPANSION:

$$g_q^+ = \partial_q e_q^- \ , \ n_q^+ = \frac{g_q^+}{\lambda^+}$$

$$g_q^- = \partial_q n_q^+ + \frac{1}{2}\partial_q^2 e_q^- = -\Lambda^+ \partial_q^2 e_q^- \ , \ n_q^- = \frac{g_q^-}{\lambda^-}$$

BOUNCE-BACK CLOSURE RELATION:

$$f_{\bar{q}}(\vec{r}_{\rm b}, t+1) = \tilde{f}_q(\vec{r}_{\rm b}, t) = f_q + g_q^+ + g_q^-$$

$$[e_q^- + \frac{1}{2}g_q^+ - \Lambda^- g_q^-](\vec{r}_{\rm b}) = 0 \ , \ e_q^- = t_q^\star(j_q + \Lambda_q^- F_q) \ , \ -F_q = \frac{\Lambda^+}{3}\partial_q^2 j_q$$

TOGETHER:

$$[j_q + \frac{1}{2}\partial_q j_q + \frac{2}{3}\Lambda \partial_q^2 j_q](\vec{r}_{\rm b}) = 0 \ , \ j_q = \rho\vec{u}\cdot\vec{c}_q \ , \ \rho\vec{u} = \sum_{q=1}^{Q-1} f_q \vec{c}_q + \frac{\vec{F}}{2} \ .$$

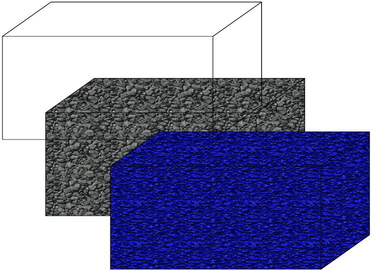
EXACT TAYLOR EXPANSION ONLY IF $\Lambda = \frac{3}{16}$ AND $\delta_q = \frac{1}{2}$

Consistency of the LBE Brinkman model

Stokes equation with the resistance force

$$\vec{F} = \frac{\nu_{br}}{\phi}\Delta\vec{u}\ , \quad \text{where} \quad \vec{F} = \mathbf{K}^{-}\nu\vec{u}$$

ϕ: porosity, K : prescribed permeability tensor



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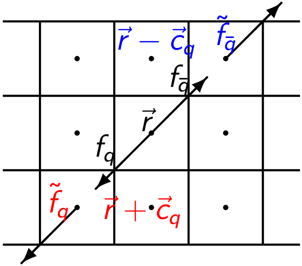
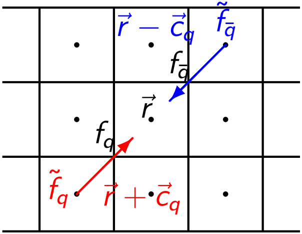
X. Nie & N. S. Martys : *"Breakdown of Chapman-Enskog expansion* and the anisotropic effect for lattice-Boltzmann models of porous media" (*Phys. Fluids*, 2007):
the apparent BGK viscosity differs from the predicted,

$$\nu_{\mathbf{br}} \neq \frac{\mathbf{\Lambda}^{+}}{\mathbf{3}}.$$

Consider **one pair of evolution equations**



and **another pair (back)**



The $L-$operator is equivalent to recurrence equations:

$$g_q^{\pm}(\vec{r}) = [\bar{\Delta}_q e_q^{\mp} - \Lambda_q^{\mp}\Delta_q^2 e_q^{\pm} + (\Lambda_q - \frac{1}{4})\Delta_q^2 g_q^{\pm}](\vec{r})$$

using the **link-wise finite-difference operators:**

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

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

The $L-$operator is equivalent to recurrence equations:

$$g_q^{\pm}(\vec{r}) \;=\; [\bar{\Delta}_q e_q^{\mp} - \Lambda_q^{\mp}\Delta_q^2 e_q^{\pm} + (\Lambda_q - \frac{1}{4})\Delta_q^2 g_q^{\pm}](\vec{r})$$

Bulk solution is:

$$g_q^{\pm}(\vec{r}) = \gamma_q(e_q^{\mp}) - 2\Lambda_q^{\mp}\Gamma_q(e_q^{\pm}) \;,$$

$\gamma_q(\phi)$ and $\Gamma_q(\phi)$ obey :

γ_q : **odd-order variation of** $\phi = e_q^{\mp}$

$$\gamma_q(\phi) \;=\; \bar{\Delta}_q\phi + (\Lambda_q - \frac{1}{4})\Delta_q^2\gamma_q(\phi) \;,$$

Γ_q : **even-order variation of** $\phi = e_q^{\pm}$

$$2\Gamma_q(\phi) \;=\; \Delta_q^2\phi + 2(\Lambda_q - \frac{1}{4})\Delta_q^2\Gamma_q(\phi) \;.$$

The $L-$operator is equivalent to recurrence equations:

$$g_q^{\pm}(\vec{r}) \;=\; [\bar{\Delta}_q e_q^{\mp} - \Lambda_q^{\mp}\Delta_q^2 e_q^{\pm} + (\Lambda_q - \frac{1}{4})\Delta_q^2 g_q^{\pm}](\vec{r})$$

Exact macroscopic equations are:

$$\sum_{q=0}^{Q-1} g_q^{+} = 0\;,\;\sum_{q=0}^{Q-1} g_q^{-}\vec{c}_q = \vec{F}$$

Steady Stokes equation

Substituting Stokes equilibrium distribution

$$j_q^\star = t_q^\star(\vec{j}\cdot\vec{c}_q)\ ,\ F_q^\star = t_q^\star(\vec{F}\cdot\vec{c}_q)\ ,\ P_q^\star = t_q^\star P(\rho)$$

Mass $\times\boldsymbol{\Lambda}^+$:

$$(\bar{\Delta}_q\Lambda^+ j_q^\star \cdot 1_q) = \Lambda(\Delta_q^2 P_q^\star \cdot 1_q)$$

$$-(\Lambda - \frac{1}{4}) \times ([\Delta_q^2\gamma_q(\Lambda^+ j_q^\star) + \Lambda\Delta_q^2\gamma_q(F_q^\star) - 2\Lambda\Delta_q^2\Gamma_q(P_q^\star)] \cdot 1_q)$$

Momentum :

$$(\bar{\Delta}_q P_q^\star \cdot \vec{c}_q) = \vec{F} + (\Delta_q^2\Lambda^+ j_q^\star \cdot \vec{c}_q) + \Lambda(\Delta_q^2 F_q^\star \cdot \vec{c}_q)$$

$$-(\Lambda - \frac{1}{4}) \times ([\Delta_q^2\gamma_q(P_q^\star) - 2\Delta_q^2\Gamma_q(\Lambda^+ j_q^\star) - 2\Lambda\Delta_q^2\Gamma_q(F_q^\star)] \cdot \vec{c}_q)$$

Parametrization of the bounce-back

EXACT STEADY STATE CLOSURE RELATION:

$$[e_q^- + \frac{1}{2}g_q^+ - \Lambda^- g_q^-](\vec{r}_{\rm b}) = 0$$

Then the closure relation becomes (multiplying by Λ^+):

$$(\Lambda^+ j_q^\star) \;+\; \Lambda F_q^\star + \frac{1}{2}(\gamma_q(\Lambda^+ j_q^\star) + \Lambda\gamma_q(F_q^\star) - 2\Lambda\Gamma_q(P_q^\star)) \\ +\; 2\Lambda(\Gamma_q(\Lambda^+ j_q^\star) + 2\Lambda\Gamma_q(F_q^\star) - \Lambda\gamma_q(P_q^\star)) = 0\,.$$

THEN BOUNCE-BACK MAINTAINS THE PROPERTIES OF BULK SOLUTION ! *And the TRT/MRT gives viscosity independent permeability for fixed* Λ *!*

From recurrence solution to Chapman-Enskog expansion

Expand the recurrence solution:

$$\begin{aligned} \gamma_q(\phi) &= \bar{\Delta}_q \phi + (\Lambda_q - \frac{1}{4})\Delta_q^2 \gamma_q(\phi) , \\ 2\Gamma_q(\phi) &= \Delta_q^2 \phi + 2(\Lambda_q - \frac{1}{4})\Delta_q^2 \Gamma_q(\phi) . \end{aligned}$$

into series around the equilibrium:

$$\gamma_q(\phi) = \sum_{k\geq 1} \frac{a_{2k-1}\partial_q^{2k-1}\phi}{(2k-1)!} , \qquad \Gamma_q(\phi) = \sum_{k\geq 1} \frac{a_{2k}\partial_q^{2k}\phi}{(2k)!} ,$$

also replacing the central-difference operators by the series:

$$\bar{\Delta}_q \psi = \sum_{k\geq 1} \frac{\partial_q^{2k-1}\psi}{(2k-1)!} , \ \Delta_q^2 \psi = 2\sum_{k\geq 1} \frac{\partial_q^{2k}\psi}{(2k)!} , \ \forall \psi .$$

From recurrence solution to Chapman-Enskog expansion

the solution of recurrence equations is:

$$\gamma_q(\phi) = \sum_{k\geq 1} \frac{a_{2k-1}\partial_q^{2k-1}\phi}{(2k-1)!} \,, \qquad \Gamma_q(\phi) = \sum_{k\geq 1} \frac{a_{2k}\partial_q^{2k}\phi}{(2k)!} \,,$$

where

$$\begin{aligned} a_1 &= 1\,,\ a_2 = 1\,, \\ a_{2k-1} &= 1 + 2(\Lambda_q - \frac{1}{4}) \sum_{1\leq n<k} a_{2n-1}\frac{(2k-1)!}{(2n-1)!(2(k-n))!}\,, \\ a_{2k} &= 1 + 2(\Lambda_q - \frac{1}{4}) \sum_{1\leq n<k} a_{2n}\frac{(2k)!}{(2n)!(2(k-n))!}\,. \end{aligned}$$

Back to Brinkman problem

The second order correction in the RHS of NSE is:

$$err(\vec{F}) = \nabla \cdot \frac{\Lambda^+}{3} \nabla \Lambda^- \vec{F}$$

Back to Brinkman problem

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The second-order error for the resistance force is:

$$err(\vec{F} = -\frac{\nu \vec{u}}{k}) = -\frac{\Lambda}{3k} \nu \Delta \vec{u}$$

Back to Brinkman problem

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The exact *effective viscosity coefficient*, **either from the recurrence equations or** *the infinite* **Chapman-Enskog expansion, for parallel** ($\Theta^2 = 1$) **and diagonal** ($\Theta^2 = \frac{1}{2}$) **flows:**

$$\nu \Longrightarrow \nu(1 - \frac{\Lambda}{3k} + \frac{\Theta^2}{k}(\Lambda - \frac{1}{4}))$$

It depends on the orientation (Θ^2 !), except for $\Lambda = \frac{1}{4}$!

Recurrence equations for time dependent problems

Exact conservation equation: $(g_q^{\pm} \cdot v_q^{\pm}) = 0$ for $\phi^{\pm} = (e_q^{\pm} \cdot v_q^{\pm})$,
$v_q^{+} = 1_q$ and $v_q^{-} = \vec{c}_q$

$$\begin{aligned} \underline{\bar{\Delta}_t \phi^{\pm} + \Lambda^{\mp} \Delta_t^2 \phi^{\pm}} &= -(\mathcal{S}_q^{\pm} \cdot v_q^{\pm}) \\ \mathcal{S}_q^{\pm}(\vec{r}, t) &= \bar{\Delta}_q e_q^{\mp} - \Lambda^{\mp} \Delta_q^2 e_q^{\pm} + (\Lambda - \frac{1}{4}) \Delta_q^2 g_q^{\pm} \end{aligned}$$

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$v_q^{+} = 1_q$ and $v_q^{-} = \vec{c}_q$

$$\bar{\Delta}_t \phi^{\pm} + \Lambda^{\mp} \Delta_t^2 \phi^{\pm} = -(\mathcal{S}_q^{\pm} \cdot v_q^{\pm})$$

$$\mathcal{S}_q^{\pm}(\vec{r}, t) = \bar{\Delta}_q e_q^{\mp} - \Lambda^{\mp} \Delta_q^2 e_q^{\pm} + (\Lambda - \frac{1}{4}) \Delta_q^2 g_q^{\pm}$$

with three-level time difference :

$$\bar{\Delta}_t \phi^{\pm} + \Lambda^{\mp} \Delta_t^2 \phi^{\pm} = (\Lambda^{\mp} + \frac{1}{2}) \phi^{\pm}(t+1) - 2\Lambda^{\mp} \phi^{\pm}(t) + (\Lambda^{\mp} - \frac{1}{2}) \phi^{\pm}(t-1)$$

Recurrence equations for time dependent problems

Equivalent diffusion equation when $\Lambda = \frac{1}{4}$ is:

$$\frac{\rho(t+1) - \rho(t-1)}{2} = \Lambda^{-} c_e \times$$

$$\sum_{q=1}^{Q-1} t_q^{(m)} (\rho(\vec{r} + \vec{c}_q, t) - (\rho(\vec{r}, t-1) + \rho(\vec{r}, t+1)) + \rho(\vec{r} - \vec{c}_q, t))$$

Recurrence equations for time dependent problems

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This is idea of Du Fort-Frankel diffusion scheme, *M.T.A.C.* 1953: *explicit and unconditionally stable* !

Recurrence equations for time dependent problems

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This is idea of Du Fort-Frankel diffusion scheme, *M.T.A.C.* 1953: *explicit and unconditionally stable* !

Optimal stability of
OTRT $= \textbf{TRT}(\Lambda = \frac{1}{4}) = \textbf{TRT}(\frac{\lambda^+ + \lambda^-}{2} = -1)$:
the same stability for any Λ^- and Λ^+ provided that $\Lambda^-\Lambda^+ = \frac{1}{4}$

Towards conclusion

The magic parameter Λ controls

1. Stability

Towards conclusion

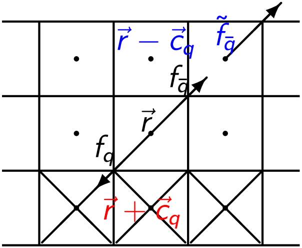
THE MAGIC PARAMETER Λ CONTROLS

1. Stability
2. Consistency and accuracy (beyond the second order) of bulk solutions at steady state
   - They are set on a given grid when Reynold/Peclet and Λ are constant !

Towards conclusion

The magic parameter Λ controls

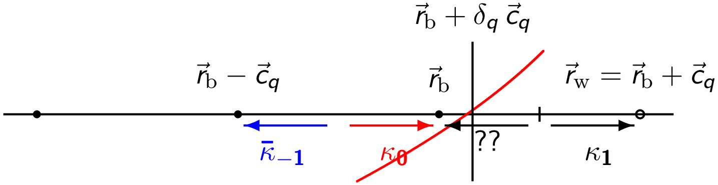
1. Stability
2. Consistency and accuracy (beyond the second order) of bulk solutions at steady state
3. The boundary/interface accomodation layers



Towards conclusion

The magic parameter Λ controls

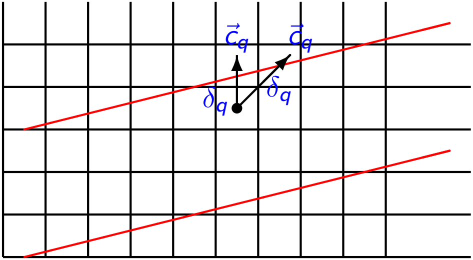
1. Stability
2. Consistency and accuracy (beyond the second order) of bulk solutions at steady state
3. There exist the *infinite number of second and third order* accurate consistent boundary schemes.



Towards conclusion

The magic parameter Λ controls

1. Stability
2. Consistency and accuracy (beyond the second order) of bulk solutions at steady state
3. The third-order accurate schemes are exact for inclined Poiseuille flow at any Λ and they shift the dependency on Λ beyond the second order.



Towards conclusion

THE MAGIC PARAMETER Λ CONTROLS

1. Stability
2. Consistency and accuracy (beyond the second order) of bulk solutions at steady state
3. The boundary/interface accomodation layers
4. A compromise between the advanced efficiency and precision is looked for:
   $\Lambda = \frac{1}{4}\ ,\ \frac{3}{16}\ ,\ \frac{1}{6}(O(h^4) = 0)\ ,\ \frac{1}{12}(O(h^3) = 0), \ldots$???
   permeability measurements in CT images better agree with the experiment when $\Lambda \to 0$...
   courtesy of Valérie Pot (INRA) and Laurent Talon (FAST)

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