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Lattice Boltzmann schemes for the *Brinkman* equation in extremely heterogeneous porous media: bulk, boundary, interface

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Groupe de travail "Schémas de Boltzmann sur réseau"

6th May 2015

Outline	Who am I?	$\mathbf{Context}$	TRT-LBM	Channels	Non-channels

- 1 Who am I?
 - PhD work
 - Experiments
 - Numerics
- 2 Context
 - Motivation
- **3** TRT-LBM
 - Properties
- 4 Channels
 - Bulk
 - Boundary/interface
 - Boundary/interface
 - Solutions
 - Conclusions
- **5** Non-channels
 - Benchmark description

Outline	Who am I?	$\mathbf{Context}$	TRT-LBM	Channels	Non-channels

- Approximated solutions
- Stokes flow around solid cylinder
- Porous flow around solid cylinder
- Conclusions
- Biporous medium: Introduction
- Porous flow across porous cylinder $k_1 \ll k_2$
- Porous flow across porous cylinder $k_1 \gg k_2$
- Conclusions

> Theoretical, numerical and experimental characterization of microfluidic channel flows in rotating platforms



Examples of lab-on-a-CD prototypes, (a) image source: Brenner et al. 2003; (b) image source:

www.spaceref.com

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Outline	Who am I?	$\mathbf{Context}$	TRT-LBM	Channels	Non-channels		
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Experiments							

Example of micro-PIV measurement



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Micro-PIV





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Centrifugal-driven rotating channel

flow setup

Streamwise pressure solution predicted by several commercial CFD codes

- image source: Glatzela et al. 2008

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Image: Image:



LBM studies:



A study on the inclusion of body forces in the lattice Boltzmann BGK equation to recover steady-state hydrodynamics

Goncalo Silva, Viriato Semiao* Mechanical Engineering Department, Instituto Superior Tecnico, Technical University of Lisbon, Av. Rovisco Pais, 1049-001 Lisbon, Portugal J. Fluid Mech., page 1 of 22. © Cambridge University Press 2012 doi:10.1017/jfm.2012.83

First- and second-order forcing expansions in a lattice Boltzmann method reproducing isothermal hydrodynamics in artificial compressibility form

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(Received 6 October 2011; revised 22 December 2011; accepted 7 February 2012)

Journal of Computational Physics 269 (2014) 259-279



Truncation errors and the rotational invariance of three-dimensional lattice models in the lattice Boltzmann method



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$\mathbf{Outline}$	Who am I?	Context	TRT-LBM	Channels	Non-channels
Numeric	s				

Results: Ek⁻¹
$$\equiv \frac{\Omega_z H^2}{\nu} = 0.001$$



(c) D3Q27





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Numerics	5				

Results: Ek⁻¹ =
$$\frac{\Omega_z H^2}{\nu} = 0.02$$

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(c) D3Q27







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Outline	Who am I?	Context	TRT-LBM 0000	$\begin{array}{c} \mathbf{Channels} \\ \texttt{0000000000} \end{array}$	Non-channels 000000000000000000000000000000000000
Numerics	s				

Results: Ek⁻¹ =
$$\frac{\Omega_z H^2}{\nu} = 0.05$$









(d)



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Results: Ek⁻¹
$$\equiv \frac{\Omega_z H^2}{\nu} = 0.1$$



(c) D3Q27







(d)



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Results:
$$\operatorname{Ek}^{-1} \equiv \frac{\Omega_z H^2}{\nu} = 1$$



(c) D3Q27







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Motivation

Heterogeneous porous media systems



Figure 1: SEM (Scanning Electron Microscope) view of used cabin automotive air filter



pure 2: SEM representing the stationary stage of dust loads

Figure 4: SDM of dust calle formation on the filter surface

Figure 3: SEM of duct loaded filter has passed the depth filtration

image source: www.ntu.edu.sg



image source: www.ntu.edu.sg



image source: www.memfil.com



Figure 2. Liquid Filtration Media

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Motivation

Governing equations (nondimensional)

 ${\bf Stokes\text{-}Brinkman\text{-}Darcy}\ equations$

$$\vec{\nabla} \cdot \vec{u} = 0$$
$$f(\phi)\vec{\nabla}p = \Delta \vec{u} - \sigma^2 \vec{u}$$

subject to proper <u>interface/solid BC</u>. Solution is controlled by:

•
$$f(\phi)$$
 (herein = 1, for simplicity)

• $\sigma^2 = f(\phi) H^2/k$

Given $\sigma \Rightarrow 3$ dynamical regimes follow:

3
$$\sigma > 1$$
: "Constant" flow $\rightarrow \underline{\text{Darcy}}$

Channel flow solutions:







- Streaming: $f_q(\vec{r} + \vec{c}_q, t+1) = \tilde{f}_q(\vec{r}, t)$
 - TRT collision: $\tilde{f}_q(\vec{r},t) = f_q(\vec{r},t) + g_q^+ + g_q^$ where $g_q^{\pm} = -s^{\pm} \left(f_q^{\pm} - e_q^{\pm} \right)$ defined by:
 - Symmetric equilibrium $e_q^+ = t_q P(\rho)$
 - Anti-symmetric equilibrium $e_q^- = j_q + \Lambda^- F_q$ with $j_q = t_q(\vec{j} \cdot \vec{c}_q)$ and $F_q = t_q(\vec{F} \cdot \vec{c}_q)$
 - Relaxation functions $\Lambda^{\pm} = \left(\frac{1}{s^{\pm}} \frac{1}{2}\right) > 0$ with $s^{\pm} \in]0, 2[$

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• Brinkman viscosity
$$\nu_B = \frac{\nu}{f(\phi)} = \frac{\Lambda^+}{3}$$



6 BF scheme:

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• Brinkman force term: $\vec{F} = \vec{F}^p - B_f \vec{j}$ with $B_f = \frac{\nu}{k}$

6 IBF scheme:

• Introduce redefine symmetric relaxation function, e.g. $\Lambda^+_* = \frac{3(4+B)\Lambda^+}{4(3+2B\Lambda)}$ where $B = \frac{\sigma^2}{H^2}$ or $B = \frac{B_f}{\nu_B}$

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• One pair of linear combinations per link:

$$\begin{split} g_q^+ &= \bar{\Delta}_q e_q^- - \Lambda^- \bar{\Delta}_q^2 e_q^+ + \left(\Lambda - \frac{1}{4}\right) \bar{\Delta}_q^2 g_q^+ \\ g_q^- &= \bar{\Delta}_q e_q^+ - \Lambda^+ \bar{\Delta}_q^2 e_q^- + \left(\Lambda - \frac{1}{4}\right) \bar{\Delta}_q^2 g_q^- \end{split}$$



2 And another pair per link:

$$\begin{split} \bar{\Delta}_q g_q^- &= \bar{\Delta}_q^2 e_q^+ - \Lambda^+ \bar{\Delta}_q^2 g_q^+ \\ \bar{\Delta}_q g_q^+ &= \bar{\Delta}_q^2 e_q^- - \Lambda^- \bar{\Delta}_q^2 g_q^- \end{split}$$

where first and second central linkwise finite differences are:

•
$$\bar{\Delta}_q \psi = \frac{1}{2} \left(\psi(\vec{r} + \vec{c}_q) - \psi(\vec{r} - \vec{c}_q) \right)$$

• $\bar{\Delta}_q^2 \psi = \psi(\vec{r} + \vec{c}_q) - 2\psi(\vec{r}) + \psi(\vec{r} - \vec{c}_q)$

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Properties								
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(General solution:)

• Exact steady macroscopic equations:

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

• Taking the moments of recurrence equations g_q^{\pm} :

$$\overline{\nabla} \cdot \vec{j} = \Lambda^{-} \overline{\Delta}^{2} P - \left(\Lambda - \frac{1}{4}\right) \sum_{q=1}^{Q-1} \overline{\Delta}_{q}^{2} g_{q}^{+}$$

$$\overline{\nabla} P - \vec{F} = \frac{\Lambda^{+}}{3} \overline{\Delta}^{2} \vec{j} + \Lambda \sum_{q=1}^{Q-1} \overline{\Delta}_{q}^{2} F_{q}^{-} \vec{c}_{q} - \left(\Lambda - \frac{1}{4}\right) \sum_{q=1}^{Q-1} \overline{\Delta}_{q}^{2} g_{q}^{-} \vec{c}_{q}$$

• $\overline{\nabla} \cdot \vec{j} = \sum_{q=1}^{Q-1} \bar{\Delta}_q j_q$ • $\bar{\Delta}^2 P = \sum_{q=1}^{Q-1} \bar{\Delta}_q^2 P_q$ • $\overline{\nabla} P = \sum_{q=1}^{Q-1} \bar{\Delta}_q P_q \vec{c}_q$ • $\bar{\Delta}^2 \vec{j} = 3 \sum_{q=1}^{Q-1} \bar{\Delta}_q^2 j_q \vec{c}_q$ • Isotropic correction (Brinkman eq.):

 $\Lambda\sum_{q=1}^{Q-1}\bar{\Delta}_q^2F_q^-\vec{c}_q=-\frac{\Lambda B_f}{3}\bar{\Delta}^2\vec{j}$

• Anisotropic correction (Brinkman eq.): $\left(\Lambda - \frac{1}{4}\right)\sum_{q=1}^{Q-1}\bar{\Delta}_{q}^{2}g_{q}^{-}\vec{c}_{q} =?$

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Bulk					

Channel solution:)

Straight/diagonal channel in rotated coordinate system (x', y'):

$$\begin{array}{l} \bullet \quad \text{Momentum: } \sum_{q=1}^{Q-1} g_q^- c_{qx'} = F_{x'} \\ \bullet \quad \text{Periodic condition: } g_q^- = 0 \text{ if } c_{qy'} = 0 \end{array} \qquad \Longrightarrow \quad \overbrace{ \begin{array}{l} g_q^- = 3t_q F_{x'}(y') c_{qx'} c_{qy'}^2 \\ \bullet \quad \end{array} } \\ \end{array}$$

Anisotropic correction (Brinkman eq.):

$$\left(\Lambda - \frac{1}{4}\right) \sum_{q=1}^{Q-1} \bar{\Delta}_q^2 g_{\bar{q}} \vec{c}_q = -3\left(\Lambda - \frac{1}{4}\right) B_f \bar{\Delta}_{y'}^2 j_{x'} \sum_{q=1}^{Q-1} t_q c_{qx'}^2 c_{qy'}^2 = -\left(\Lambda - \frac{1}{4}\right) B_f \bar{\Delta}_{y'}^2 j_{x'}$$

Total correction (Isotropic+Anisotropic):

$$-\frac{\Lambda B_f}{3}\bar{\Delta}_{y'}^2 j_{x'} + \left(\Lambda - \frac{1}{4}\right) B_f \bar{\Delta}_{y'}^2 j_{x'} = B_f \left(\frac{8\Lambda - 3}{12}\right) \bar{\Delta}_{y'}^2 j_{x'}$$

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Bulk					

Channel solution:)

Brinkman forcing modifies effective viscosity of Laplacian term

$$\overline{\nabla}_{x'}P - F_{x'} = \frac{\Lambda^+}{3}\rho_0 \left(1 + \delta\right) \bar{\Delta}_{y'}^2 u_{x'}$$

where
$$\delta = B\left(\frac{8\Lambda-3}{12}\right)$$
 with $B = \frac{3B_f}{\Lambda^+}$

Observations:

- Consistency requires viscosity independent solutions. Impossible for BGK since $\Lambda = (\tau - \frac{1}{2})^2$ makes $\delta(B, \nu)!$
- No numerical oscillations require $\delta > -1$, straight channel: $B < \frac{12}{3-8\Lambda}$.
- Idea of IBF, giving $\Lambda^+ = 3\nu_B$, $B_f = \nu/k$ and Λ , redefine: $\Lambda^+ \to \Lambda^+_* (\nu_B, B_f, \Lambda)$. Example, $\Lambda^+_* = \frac{9(4+B)\nu_B}{4(3+2B\Lambda)}$ makes $\delta = 0$.



(Solid wall:)

• Bounce-back: $f_q(\vec{r}_b, t+1) = \tilde{f}_{\bar{q}}(\vec{r}_b, t)$ with $\vec{c}_{\bar{q}} = -\vec{c}_q$ and $\vec{r}_b + \vec{c}_q \in$ solid



For a straight channel of width H, the bounce-back closure relation reads:

$$u_x \pm \frac{1}{2}\alpha^+ \bar{\Delta}_y u_x + \frac{1}{8}\alpha^- \bar{\Delta}_y^2 u_x \big|_{y_{\text{wall}} = \pm \frac{H}{2} \pm \frac{1}{2}} = 0$$

with $\alpha^+ = (1 + \delta)$ and $\alpha^- = (1 + \delta)\frac{16}{3}\Lambda$ (different coefficient values for IBF)



For stratified channels the steady-state closure relation for the (implicit) interface reads:

$$\begin{aligned} \|\nu_i(\bar{\Delta}_y u_x^{(i)} \pm \frac{1}{2}\bar{\Delta}_y^2 u_x^{(i)})\|_{Y_i \mp \frac{H}{2}} &= 0, \quad \nu_i = \nu_B^{(i)}(1+\delta_i), \\ \|u_x^{(i)} \pm \frac{1}{2}\alpha^+ \bar{\Delta}_y u_x^{(i)} + \frac{1}{8}\alpha^- \bar{\Delta}_y^2 u_x^{(i)}\|_{Y_i \mp \frac{H}{2}} &= 0 \end{aligned}$$

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with $\alpha^+ = (1 + \delta)$ and $\alpha^- = (1 + \delta)\frac{16}{3}\Lambda$ (different coefficient values for IBF)



Bounded channel

Solutions width H = 8 with $\Lambda = \left\{\frac{1}{512}, \frac{3}{16}, \frac{3}{8}, 2\right\}$



Image: Image:





Gonçalo Silva



Outline	Who am I?	Context	TRT-LBM	Channels	Non-channels			
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Conclusions								

Brinkman flow in bounded channels: boundary condition

- Physical solution experiences three regimes: Stokes, Brinkman, Darcy.
- Discrete solution is controlled by <u>bulk</u> and <u>boundary</u> approximations.
- Bulk error in BF is vanished for $\Lambda = 3/8$. For $\Lambda < 3/8$ may lead to wiggles in bulk solution. Bulk error is absent by construction in IBF.
- Bounce-back boundary error is always present (already at the 1st order) for $B \neq 0$ (when B = 0, it is exact for $\Lambda < 3/16$).
- <u>Bounce-back</u> prescribes boundary <u>implicitly</u>. It allows smoother bulk accommodation on wall. Enforcement on wall nodes triggers oscillations, e.g. FEM.

Brinkman flow in layered channels: interface condition

- Discrete solution is controlled by <u>bulk</u> and <u>interface</u> approximations.
- <u>Implicit interface prescription</u> may lead to <u>jumps</u> in continuity conditions.
- Interface continuity is only exact for B = 0 (Stokes). Interface jumps increase for $B \gg 1$ (Darcy). They decrease for $\Lambda \ll 1$, but produce wiggles. Solution: IBF.



Approximated solutions

Cell model:



General solution (Brinkman):

Main features:

- Ratio of particle to cell volume c remains invariant
- Independent of packing arrangement (in principle requires $c \ll 1$)
- Approximation on outer BC: $\overline{\omega} = 0$ (Kuwabara model)
- Polar coordinates: $(x, y) \mapsto (r, \theta)$
- Streamfunction formulation: $u_r = \frac{1}{r} \frac{\partial \psi}{\partial \theta}$ and $u_\theta = -\frac{\partial \psi}{\partial r}$

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$$\psi^{(i)}(r,\theta) = \left(\frac{C_1^{(i)}}{r} + C_2^{(i)}r + C_3^{(i)}I_1(\sigma_1 r) + C_4^{(i)}K_1(\sigma_1 r)\right)\sin(\theta)$$

subject to proper interface/solid BC

Approximated solutions

Lubrication theory:



General solution (Brinkman):

Main features:

- Ratio of particle to cell volume c remains invariant
- Depends on packing arrangement
- <u>Approximation in bulk</u>: flow asymptotically unidirectional (Lubrication model)
- Caution: singular behaviour when $H/2 - a \rightarrow 0$

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$$u_x^{(i)}(y) = -\frac{1}{\sigma_i^2} \frac{\mathrm{d}p}{\mathrm{d}x} + C_1^{(i)} \exp(y\sigma_i) + C_2^{(i)} \exp(-y\sigma_i)$$

subject to proper interface/solid BC



Permeability computations:

Cell model

$$F = \int_{0}^{2\pi} \left(\left(-p^{(2)} + \tau_{rr}^{(2)} \right) \cos\left(\theta\right) - \tau_{r\theta}^{(2)} \sin\left(\theta\right) \right)_{r=b} b \, \mathrm{d}\theta$$
$$k_{eff} = \frac{U_0}{F/V} = \frac{U_0 \, \pi b^2}{F}$$

Lubrication theory

$$Q = \int_0^{a(x)} u_x^{(1)} \, \mathrm{d}y + \int_{a(x)}^{H/2} u_x^{(2)} \, \mathrm{d}y = \frac{-f(x)}{\mu} \frac{\mathrm{d}p}{\mathrm{d}x}$$
$$k_{eff} = \frac{4a}{H} \left(\int_0^a \frac{1}{f(x)} \, \mathrm{d}x \right)^{-1}$$

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Domain discretization



Solid cylinder is discretized in a regular grid by *bounce-back* (i.e. as staircase shape), introducing a discretization error of $O(N^{-1})$

Note: Numerical solutions are evaluated for one half gap size – $N_{1/2}$



Effect of lattice resolution on accuracy



is <u>non-monotonic</u> and with large dependency on Λ at coarse resolutions



For fixed lattice resolution Λ controls Stokes solution accuracy through the location of *bounce-back* solid boundary

Remarks:

- $\underbrace{ \text{Staircase}}_{\text{diameter}} \text{ representation of cylinder reduces its true hydraulic} \\ \hline \\ \hline \\ \text{diameter} \Rightarrow \text{makes permeability solution converge to a smaller value}$
- ② <u>Large Λ </u> reduces hydraulic diameter of cylinder ⇒ under-estimates permeability at fixed grid resolution, i.e. $\frac{\partial \operatorname{err}(\mathbf{k})}{\partial \Lambda}|_{N} > 0$



Stokes flow around solid cylinder

Effect of lattice resolution on accuracy



becomes monotonic taking difference between any two Λ solutions

• Spatial convergence rate is between 1st – and 2nd – order













Outline

Who am I?

Context

TRT-LBM

Channels

Non-channels



Essentially similar to TRT Stokes solver $\Rightarrow \Lambda$ controls the accuracy through the location of *bounce-back* solid boundary

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Brinkman correction (in bulk and boundary) now plays a role \Rightarrow smaller influence of Λ over accuracy (compared to Stokes)

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Accuracy becomes independent of Λ except at small Λ values

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Effect of lattice resolution on accuracy



 $\forall \sigma$ spatial convergence rate between 1st- and 2nd-order (Data shown for BF model)

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Outline	Who am I?	Context	TRT-LBM	Channels	Non-channels			
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Conclusions								

Stokes flow around solid cylinder

- Role of Λ controls the location of the bounce-back solid boundary (by varying the size of cylinder)
- Dependency on Λ is larger at coarser lattice resolutions
- Dependency on lattice resolution indicates spatial convergence rate between 1st- and 2nd-order

Porous flow around solid cylinder

- 3 physical regimes: Stokes $\sigma \ll 1$, Brinkman $\sigma \sim O(1)$, Darcy $\sigma \gg 1$
- Stokes regime: role of Λ controls the location of the bounce-back solid boundary \Rightarrow accuracy is worst and larger dependency on Λ
- Brinkman regime: role of Λ controls both bulk and boundaries errors (Brinkman correction). Better accuracy for k. Yet, velocity solutions may experience wiggles \Leftarrow IBF corrects them \odot
- Darcy regime: role of Λ tends to cease, except at small Λ values
- Effect of lattice resolution indicates spatial convergence rate between 1^{st} and 2^{nd} -order $\forall \sigma$ regimes



1) Porous cylinder is <u>less</u> permeable than outside porous medium

 $\underbrace{\frac{k_1}{k_2} < 1}$

2) Porous cylinder is <u>more</u> permeable than outside porous medium







In both cases, **interface** continuity conditions are set *implicitly* and approximate a *staircase* cylinder



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 $\forall \sigma$ spatial convergence rate between 1st- and 2nd-order (Data shown for BF model)

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 $u_x(y)$ at vertical ($\theta = 90^\circ$) midplane for $\frac{k_1}{k_2} = 1000$ and c = 0.2



 $u_x(x)$ at horizontal ($\theta = 0^\circ$) midplane for $\frac{k_1}{k_2} = 1000$ and c = 0.2









 $u_x(y)$ at vertical ($\theta = 90^\circ$) midplane for $\frac{k_1}{k_2} = 1000$ and c = 0.7



 $u_x(x)$ at horizontal ($\theta = 0^\circ$) midplane for $\frac{k_1}{k_2} = 1000$ and c = 0.7









Effect of Λ on accuracy for $\frac{k_1}{k_0} = 1000$



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Effect of lattice resolution on accuracy for $\frac{k_1}{k_2} = 1000$



 $\forall \sigma$ spatial convergence rate between 1st- and 2nd-order (Data shown for BF model)

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Outline	Who am I?	Context	TRT-LBM	Channels	Non-channels			
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Conclusions								

Biporous medium: $k_1 \ll k_2$

- Solutions behave, approximately, as case of Brinkman flow around solid cylinder.
- However, with interface playing the role of boundary we recover larger errors (particularly in Brinkman regime).
- TRT velocity solutions are *over-estimated*, except for small Λ
- $\bullet\,$ Small Λ values lead to wiggles velocity solution profiles. They are partially corrected by IBF
- Dependency on lattice resolution indicates spatial convergence rate between 1st- and 2nd-order

Biporous medium: $k_1 \gg k_2$

- TRT velocity solutions are significantly over-estimated in Darcy regime. Solution requires use of small Λ
- However, small Λ values produce *strong* wiggles in velocity profiles. They are successfully corrected by IBF
- Dependency on lattice resolution indicates spatial convergence rate between 1st- and 2nd-order