Partially Bounce-Back method in Palabos and application to porous media

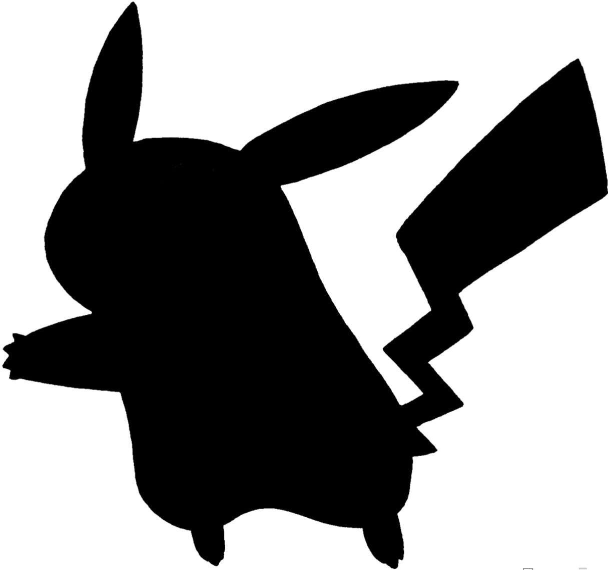
Remy Petkantchin

Palabos Summer School 2021

June 7^{th} 2021

Outline

Motivation: Curved Boundaries



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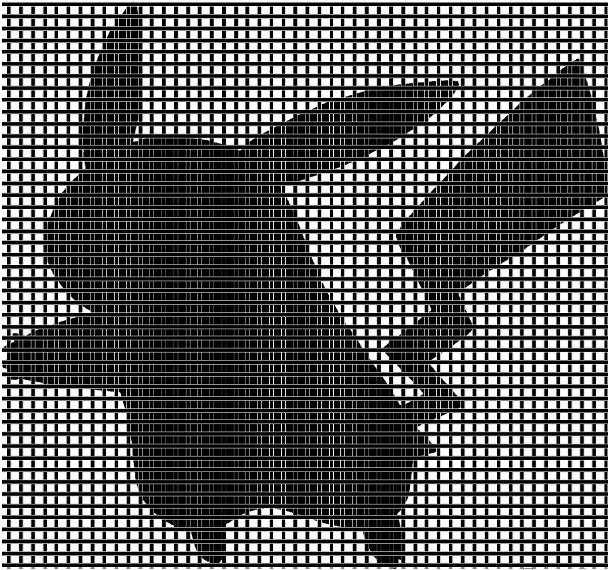

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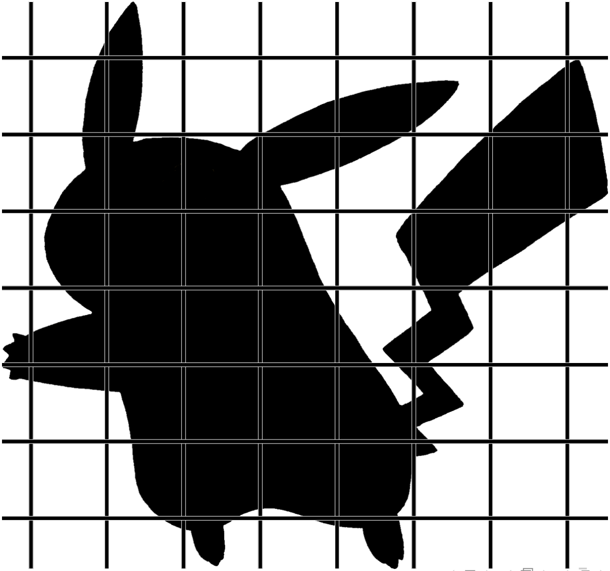

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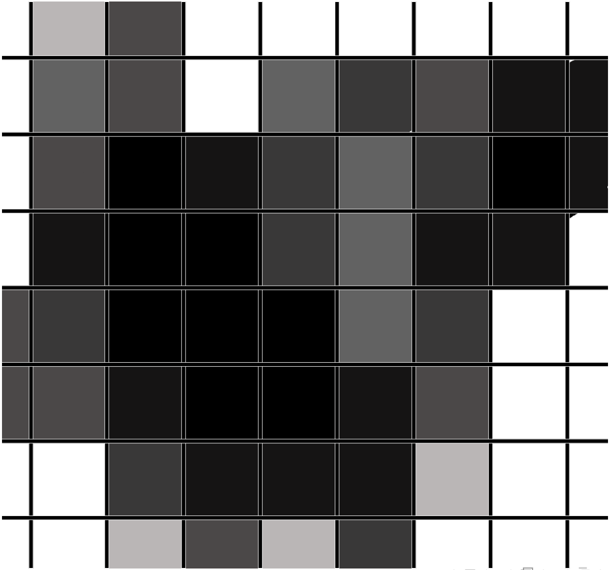

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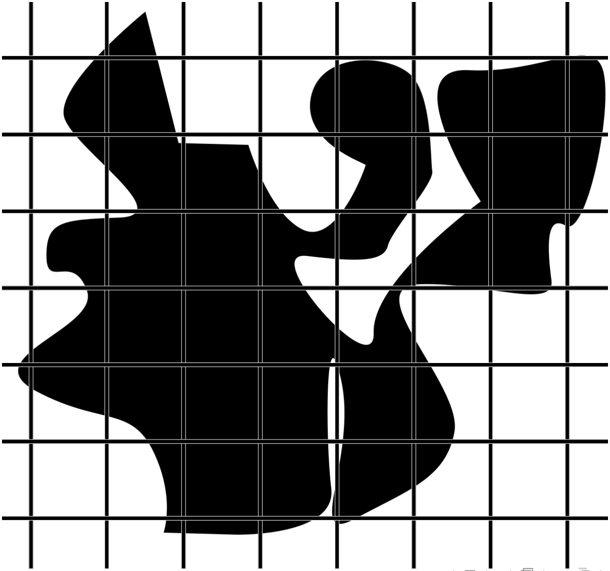
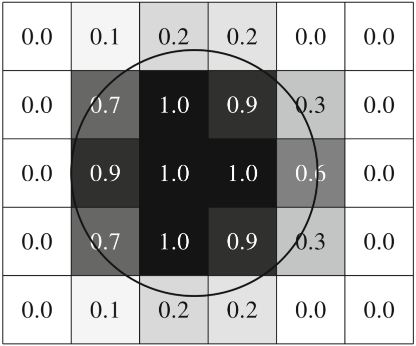
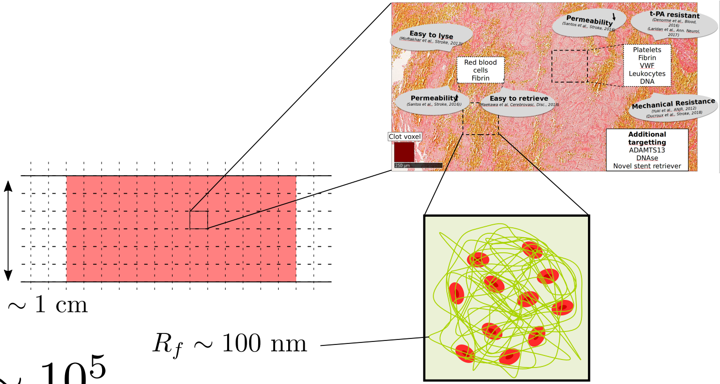


Motivation: Curved Boundaries

Fig. 11.6 Partially saturated bounce-back. A spherical particle (*circle*) covers a certain amount of each lattice cell. White corresponds to no coverage, black to full coverage. The solid fraction $0 \leq \epsilon \leq 1$ for each cell is shown up to the first digit. Lattice nodes (not shown here) are located at the centre of lattice cells



Motivation: Porous Media



$D_A \sim 1$ cm

$R_f \sim 100$ nm

$\sim 10^5$

Curved Boundaries

Original LB model [1]

$$f_i^{out}(\mathrm{x}, t) = f_i(\mathrm{x}, t) + (1 - B)\Omega_i^f + B\Omega_i^s$$

- Ω_i^f : standard BGK operator,
- $\Omega_i^s = (f_{\hat{i}}(\mathrm{x}, t) - f_{\hat{i}}^{eq}(\rho, \mathrm{u}) - (f_i(\mathrm{x}, t) - f_i^{eq}(\rho, \mathrm{u_b})$: solid collision,
- $B = \frac{\gamma(\tau - \frac{1}{2})}{(1-\gamma)+(\tau-\frac{1}{2})}$: weighting factor, γ : solid fraction.

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A LATTICE-BOLTZMANN METHOD FOR PARTIALLY SATURATED COMPUTATIONAL CELLS*

D. R. NOBLE† and J. R. TORCZYNSKI‡
Sandia National Laboratories, Albuquerque, NM 87185-0826, USA
†*E-mail: drnoble@sandia.gov*
‡*E-mail: jrtorcz@sandia.gov*

Accepted 10 October 1998

The lattice-Boltzmann (LB) method is applied to complex, moving geometries in which computational cells are partially filled with fluid. The LB algorithm is modified to include a term that depends on the percentage of the cell saturated with fluid. The method is useful for modeling suspended obstacles that do not conform to the grid. Another application is to simulations of flow through reconstructed media that are not easily segmented into solid and liquid regions. A detailed comparison is made with FIDAP simulation results for the flow about a periodic line of cylinders in a channel at a nonzero Reynolds number. Two cases are examined. In the first simulation, the cylinders are given a constant velocity along the axis of the channel, and the steady solution is acquired. The transient behavior of the system is then studied by giving the cylinders an oscillatory velocity. For both steady and oscillatory flows, the method provides excellent agreement with FIDAP simulation results, even at locations close to the surface of a cylinder. In contrast to step-like solutions produced using the "bounce-back" condition, the proposed condition gives close agreement with the smooth FIDAP predictions. Computed drag forces with the proposed condition exhibit apparent quadratic convergence with grid refinement rather than the linear convergence exhibited by other LB boundary conditions.

Keywords: Lattice-Boltzmann; Boundary Conditions; Suspensions.

Porous Media

Original LB model [2]

$$f_i^{out}(x, t) =$$
$$f_i^{c}(x, t) - \gamma f_i^{in}(x, t) + \gamma f_{\hat{i}}^{out}(x, t - \Delta t)$$

PHYSICAL REVIEW E VOLUME 57, NUMBER 4 APRIL 1998

Lattice Boltzmann scheme with real numbered solid density for the simulation of flow in porous media

Orla Dardis and John McCloskey
School of Environmental Studies, University of Ulster, Coleraine, Northern Ireland

(Received 16 June 1997)

A modified lattice Boltzmann scheme for the simulation of flow in porous media is introduced, where momentum loss due to the presence of solid obstacles to flow is incorporated into the evolution equation. A real numbered parameter specified at each lattice node is related to the density of solid scatterers and represents the effect of porous medium solid structure on hydrodynamics. This scheme removes both the need for spatial and temporal averaging and the microscopic length scales associated with important classes of porous media. A numerical study demonstrates the adherence of the approach to the Navier-Stokes equation with an effective damping term. The potential use of the scheme to aid permeability predictions in realistic geological materials is discussed. [S1063-651X(98)08404-9]

PACS number(s): 47.55.Mh, 47.11.+j, 47.15.−x

Porous Media

- Gao, Sharma (1994, LGA) [3]
- Dardis, McCloskey (1998) [1]
- Thorne, Sukop (2004) [4]
- Walsh et al. (2009) [5]
- Zhu, Ma (2013) [6]

Porous Media

- Gao, Sharma (1994, LGA)
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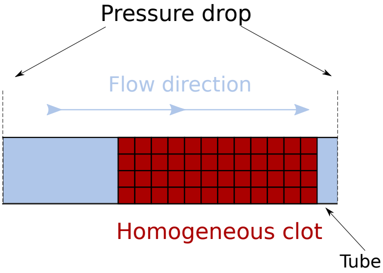
- Thorne, Sukop (2004)
- **Walsh et al. (2009) [5]**
- Zhu, Ma (2013)

Reminder: Darcy permeability

$$v_{seep} = -\frac{k}{\mu}\nabla P$$

μ : dynamic viscosity,
k : permeability.



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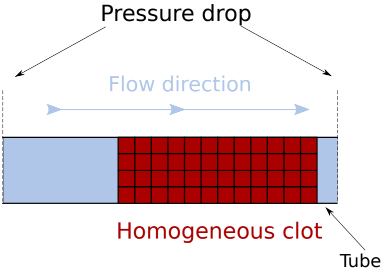

- Permeability $\leftrightarrow$ flow $\neq$ Porosity $\leftrightarrow$ structure.

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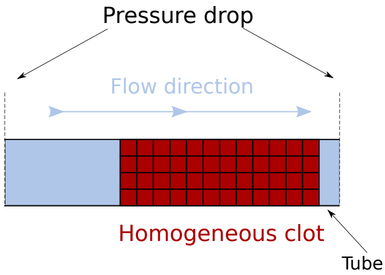

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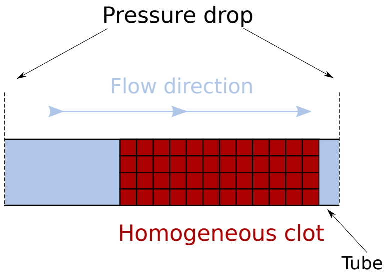
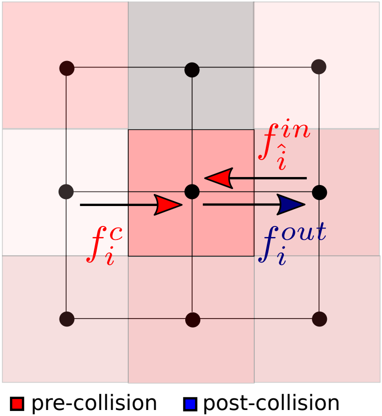


- Permeability $\leftrightarrow$ flow $\neq$ Porosity $\leftrightarrow$ structure.
- $k = k(\gamma, ...)$: permeability law
- *Assumption*: k is the macroscopic link between PBB model and reality.

Walsh PBB



$$f_i^{out}(x,t) = (1-\gamma) f_i^c(x,t) + \gamma f_{\hat{i}}^{in}(x,t)$$

Walsh PBB

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$$\rho = \sum_i f_i^{out} \qquad \rho \mathbf{u} = \sum_i f_i^{out} \mathbf{c}_i$$

Walsh PBB

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$$\rho = \sum_i f_i^{out}$$

$$\rho \mathrm{u} = \sum_i f_i^{out} \mathrm{c_i}$$

$$\rho \tilde{\mathrm{u}} = (1-\gamma) \sum_i f_i^{out} \mathrm{c_i} = (1-\gamma)\mathrm{u}$$

$\tilde{\mathrm{u}}$: macroscopic velocity.

Walsh PBB

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$$\rho \tilde{\mathrm{u}} = (1-\gamma) \sum_i f_i^{out} \mathrm{c_i} = (1-\gamma)\mathrm{u}$$

$\tilde{\mathrm{u}}$: macroscopic velocity.

Inherent permeability:

$$k = \frac{(1-\gamma)\nu}{2\gamma},$$

ν : kinematic viscosity.

Walsh PBB: Permeability Law

$$k = \frac{(1-\gamma)\nu}{2\gamma} \tag{1}$$

We have to turn this default permeability into the desired permeability law.

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$k = k(\gamma)$ and $\gamma = \gamma(n_s^*)$, with n_s^* : physical solid fraction.

Walsh PBB: Permeability Law

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$\Rightarrow k = k(\gamma) = k(n_s^*)$.

Walsh PBB: Permeability Law

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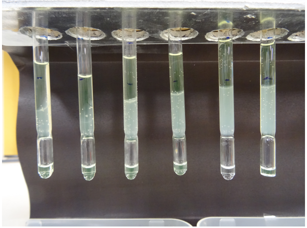
$k = k(\gamma)$ and $\gamma = \gamma(n_s^*)$, with n_s^* : physical solid fraction.
$\Rightarrow k = k(\gamma) = k(n_s^*)$.
We thus invert (1):

$$\gamma = \frac{1}{1 + \frac{2k(n_s^*)}{\nu}} \tag{2}$$

Walsh PBB

- Equivalent to Guo Force [7]
- Conserves mass and Darcy velocity in heterogeneous porous media [8]
- $k = k(\nu)$, as in all PBB models [8]

Hands-on: *in-vitro* fibrinolysis



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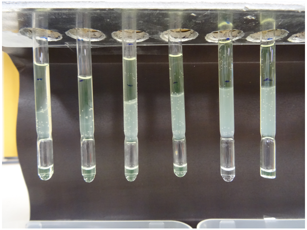

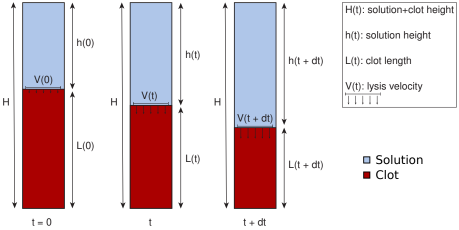

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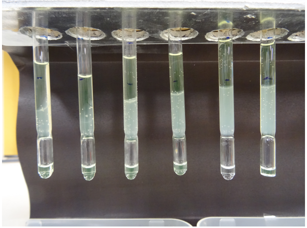

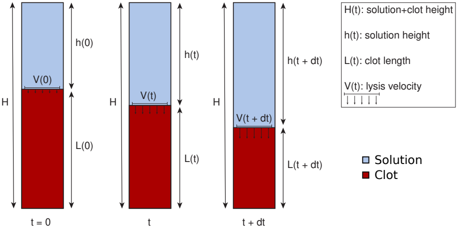

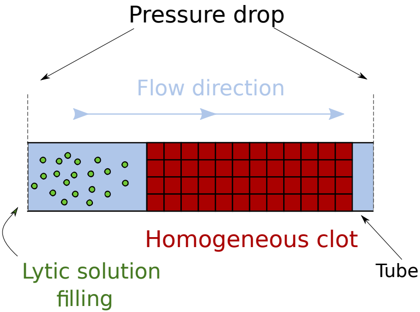

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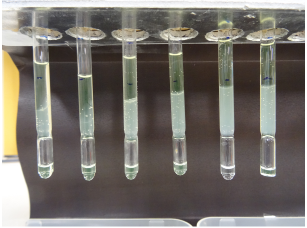
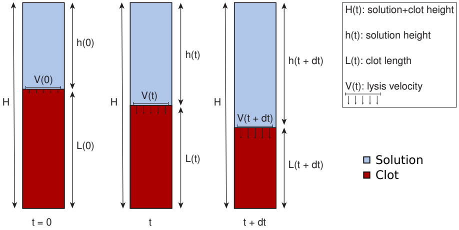
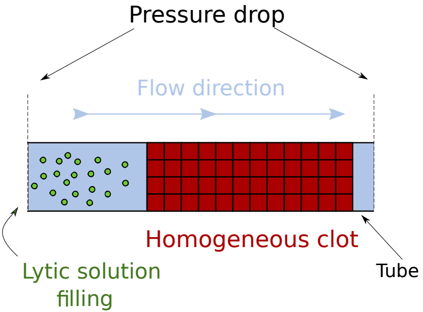






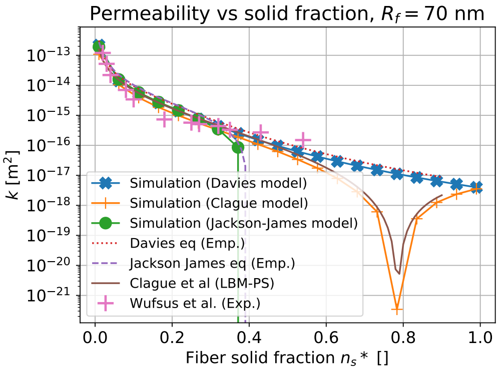
$$dFn = -k_1 Fn\tilde{Fn} \cdot dt$$

$$d\tilde{Fn} = -k_2 Fn\tilde{Fn} \cdot dt$$

and $\gamma = \gamma(Fn) \Rightarrow k = k(Fn)$.

Hands-on: *in-vitro* fibrinolysis

$$k_{Davies} = R_f^2 \left(16 n_s^{*1.5}(1 + 56 n_s^* 3)\right)^{-1} \tag{3}$$



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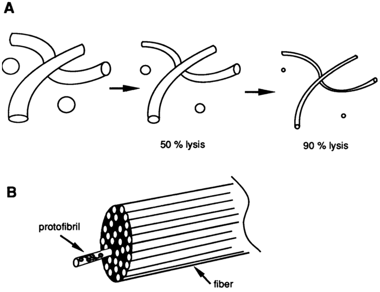

$$n_s^*(x,t) = \pi R_f(x,t)^2 \frac{L_{\Delta V}}{\Delta V}$$

Hands-on: *in-vitro* fibrinolysis

Code:
palabos/src/boundaryCondition/partialBBdynamics.hh
Exercise:
palabos/examples/showCases/partialBounceBack/README.md.pdf

Let's play!

...but any questions before?
Thanks for listening.

Refs I

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