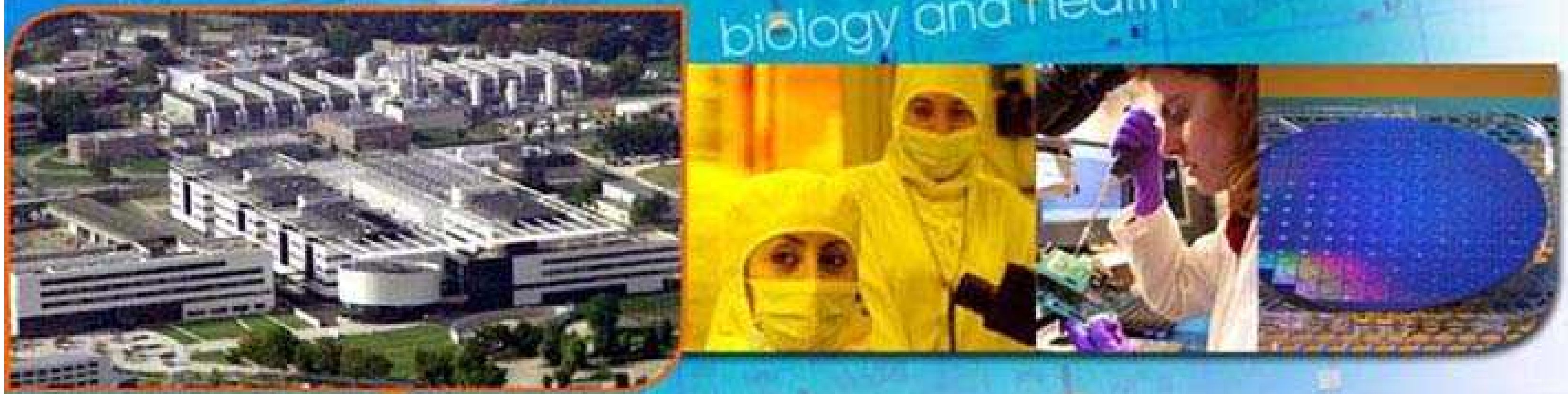
Presented at the COMSOL Conference 2008 Hannover

micro and nanoelectronics
microsystem
ambient intelligence
image chain
biology and health



2008

Interfacing continuum and discrete methods: convective diffusion of microparticles and chemical species in microsystems

J. Berthier

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Contents

- Diffusion of species, nanoparticles, macromolecules in microfluidics
    - Model
    - Applications to diffusion in cellular networks
- Convective transport
    - Model: interfacing COMSOL (carrier fluid flow field) and Monte-Carlo (particles)
    - Applications :
        - transport in a straight channel
        - recirculation regions for particle trapping
        - flow past micropillars
        - flow through a micro/nano aperture
- Conclusions and perspectives

Modeling diffusion at the microscale: the Monte-carlo approach

- Starting point: Langevin's equation
  (Newton's equation + stochastic term)
- Mimic of the random walk (*l* << *L*)
- Geometry description
- Boundary conditions

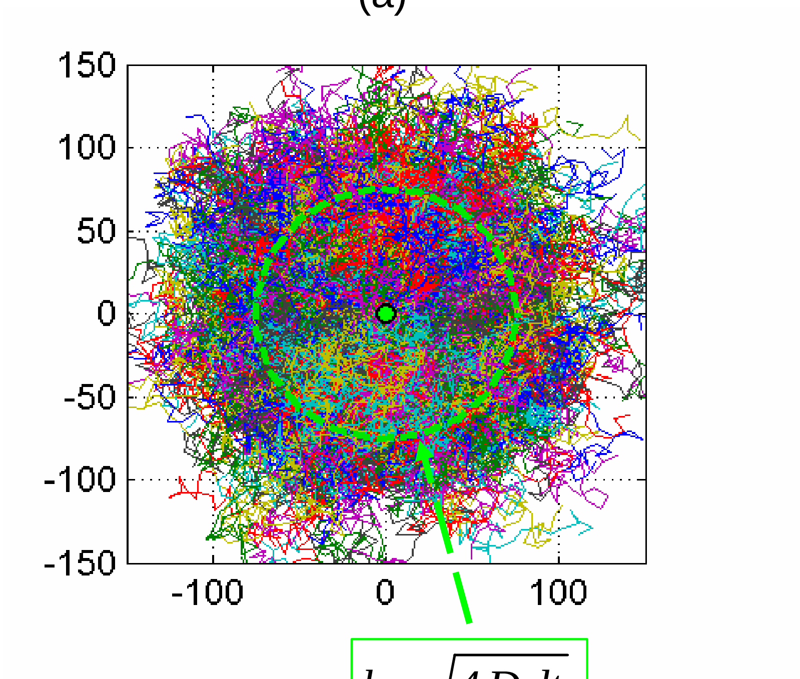
2D

$$X_{i+1} = X_i + \sqrt{4\,D\,\Delta t}\,\cos(\alpha)$$
$$Y_{i+1} = Y_i + \sqrt{4\,D\,\Delta t}\,\sin(\alpha)$$
$$\alpha = random\ (0, 2\pi)$$

3D

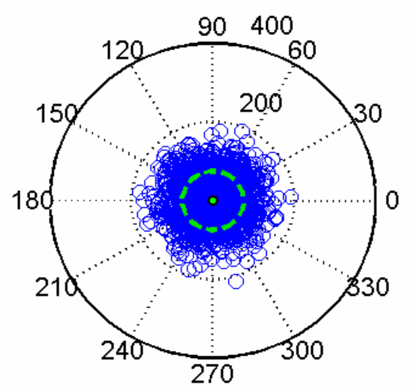
$$X_{i+1} = X_i + \sqrt{4\,D\,\Delta t}\,\cos(\alpha)\,\sin(\beta)$$
$$Y_{i+1} = Y_i + \sqrt{4\,D\,\Delta t}\,\sin(\alpha)\,\sin(\beta)$$
$$Z_{i+1} = Z_i + \sqrt{4\,D\,\Delta t}\,\cos(\beta)$$
$$\alpha = random\ (0, 2\pi)$$
$$\beta = a\cos\left(1 - 2\ random(0,1)\right)$$

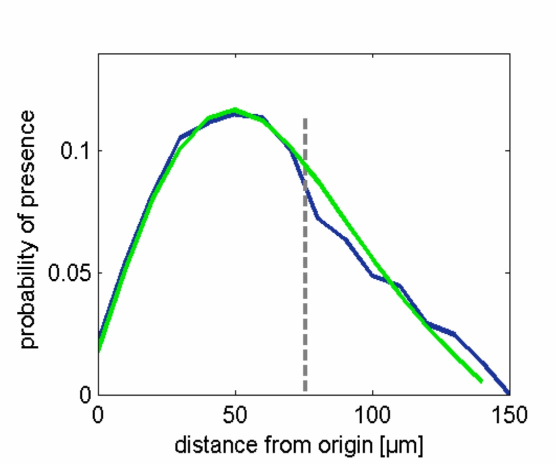
(a)



$$l = \sqrt{4\,D\,dt}$$

(b)

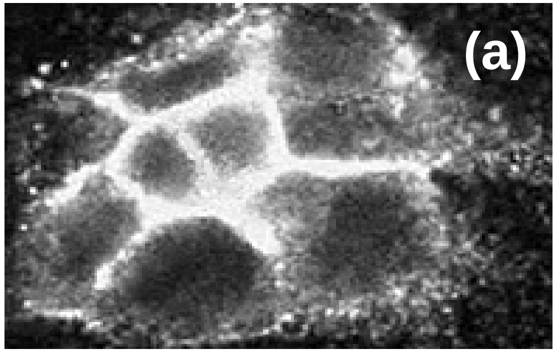




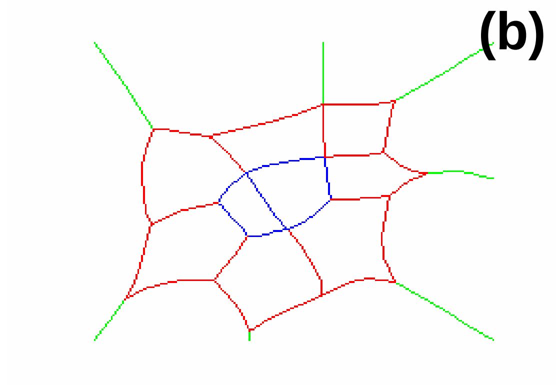
Comparison between COMSOL and Monte-Carlo model

In-vivo application: modeling diffusion in extra-cellular spaces
Application to cellular uptake

Fluorescent image of a cellular network



Schematic of the network



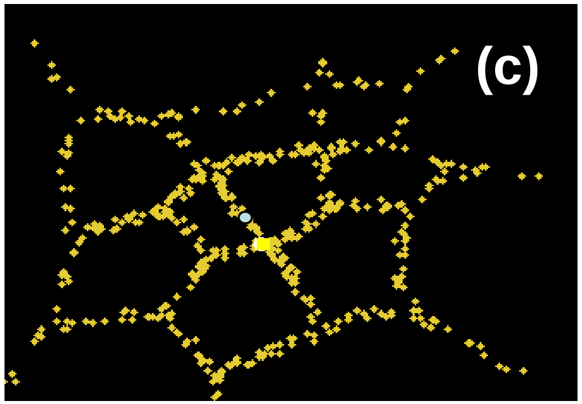
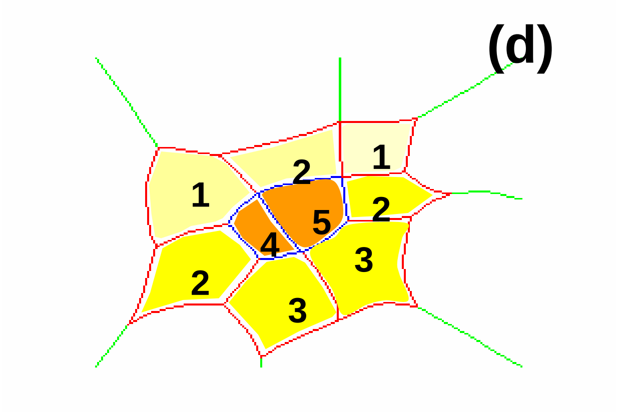


Image of the calculated network after 10 mn



Cellular uptake rate after 10 mn

Modeling diffusion at the microscale: the Monte-carlo approach

- Carrier fluid is a continuum (*Kn* ~1 → *l* ~ 10 nm for a liquid)
- Transported species may be in a discrete quantity
- Starting point: Langevin's equation
- Geometry description + boundary conditions

2D

$$X_{i+1} = X_i + V_{x,i}\,\Delta t + \sqrt{4 D \Delta t}\cos(\alpha)$$
$$Y_{i+1} = Y_i + V_{y,i}\,\Delta t + \sqrt{4 D \Delta t}\sin(\alpha)$$
$$\alpha = random\ (0, 2\pi)$$

3D

$$X_{i+1} = X_i + V_{x,i}\,\Delta t + \sqrt{4 D \Delta t}\cos(\alpha)\sin(\beta)$$
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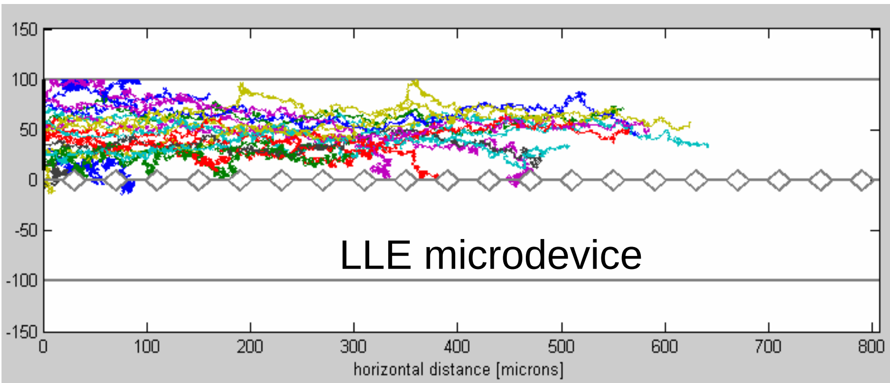
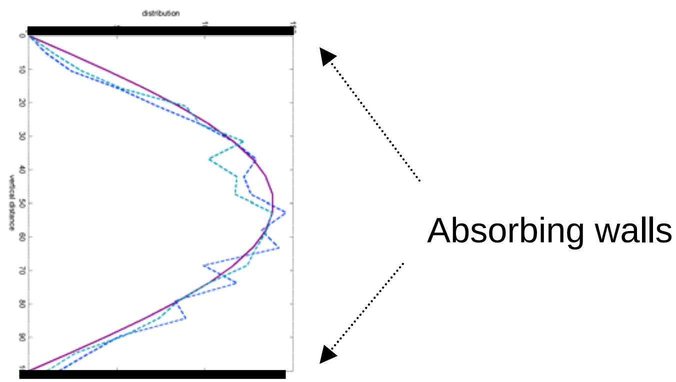
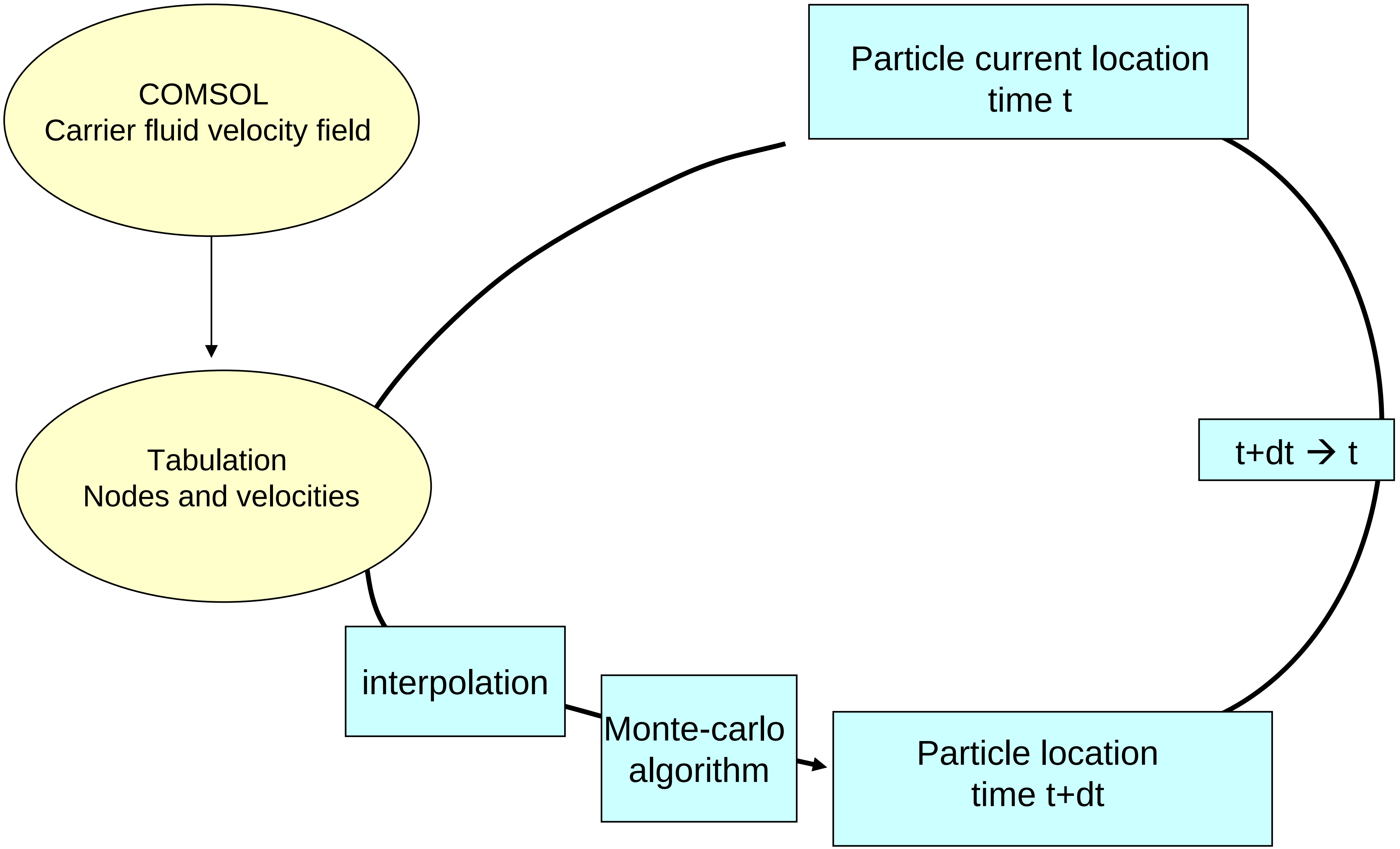


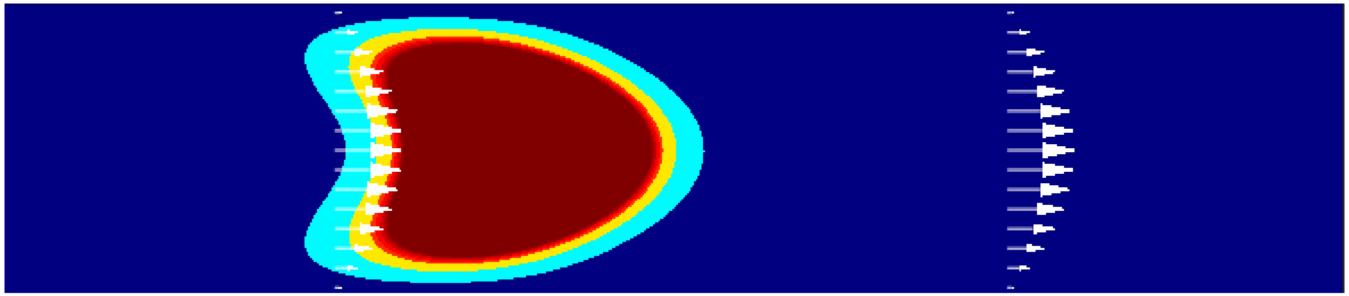


J. Berthier et al., "The physics of a coflow micro-extractor: interface stability and optimal extraction length," Sensors and Actuators A, in print.

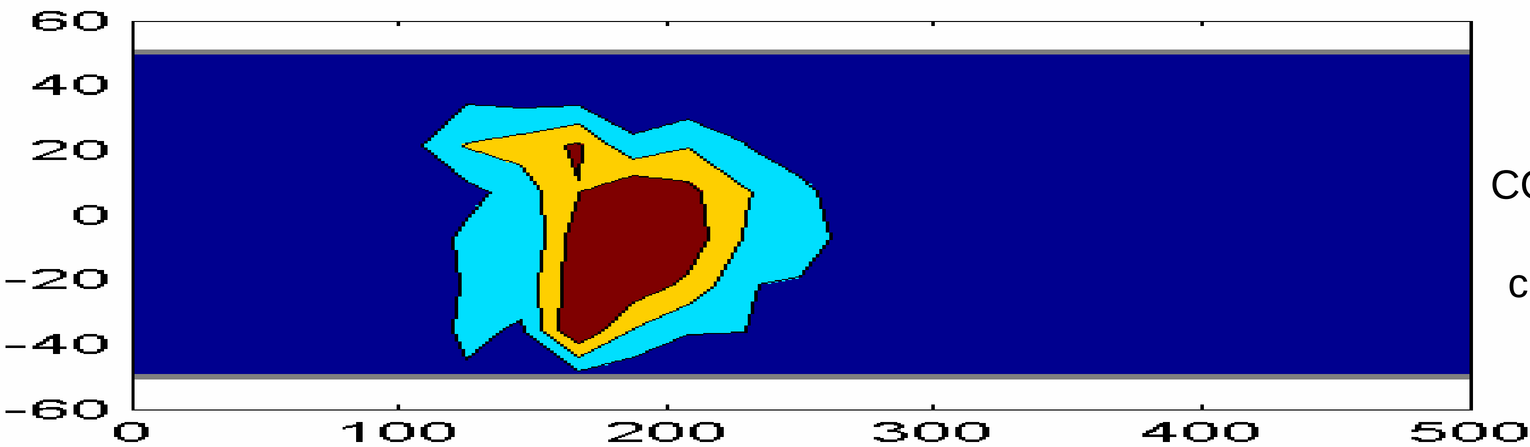
Schematic of the numerical approach



Assessment of the method in the geometry of a straight channel



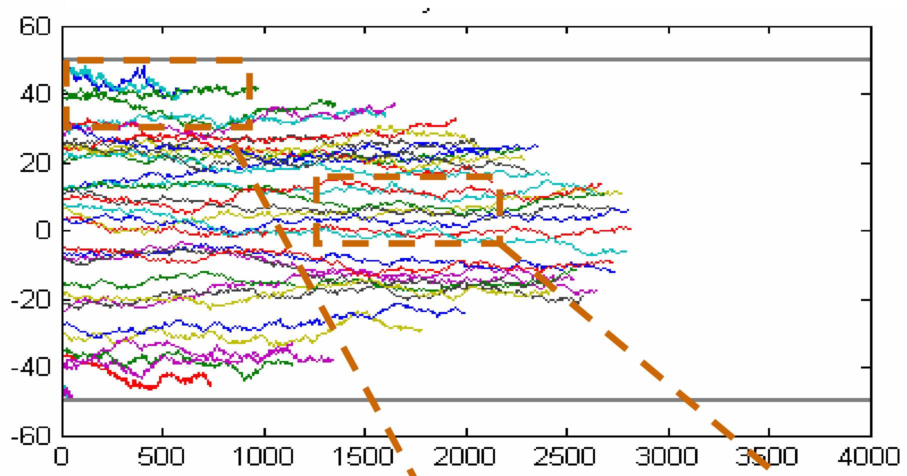
COMSOL (velocity field
+ convective transport)



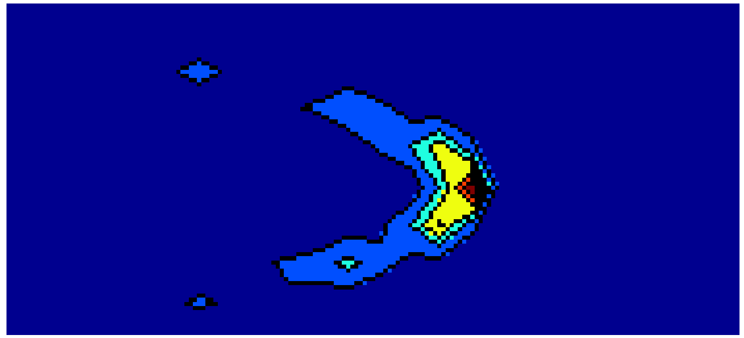
COMSOL velocity field
+ Monte-Carlo
convective transport
(200 particles)

Convective diffusion in a straight channel - viscoelastic liquid

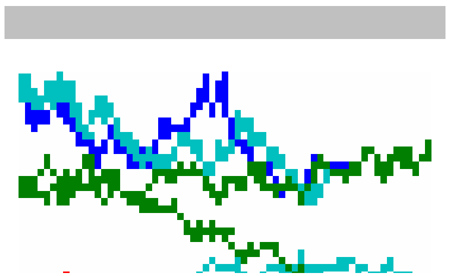
Ballistic random walk of particulates



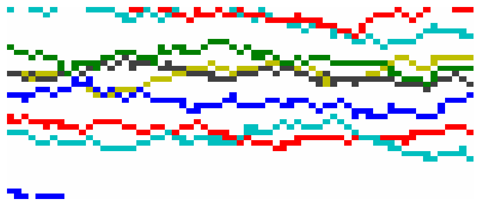
Concentration after 7 mm transport



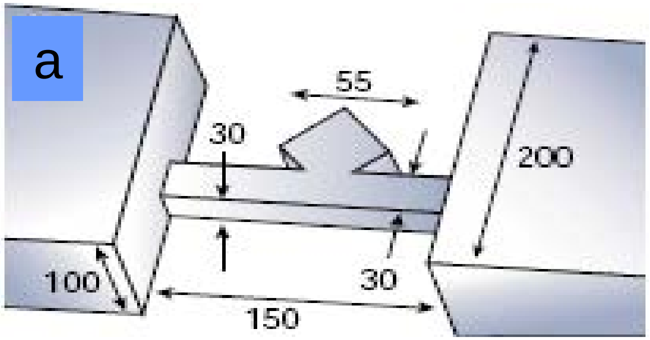
Random walk near the wall
(large shear rate)

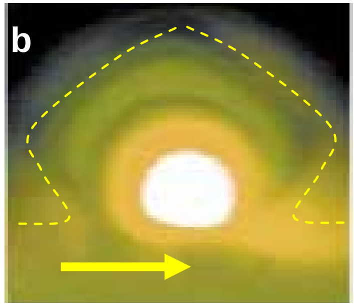


Random walk in the channel middle
(small shear rate)

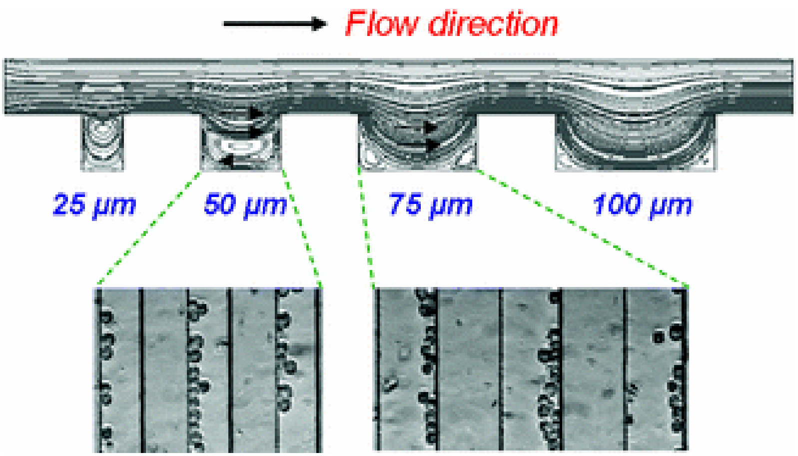


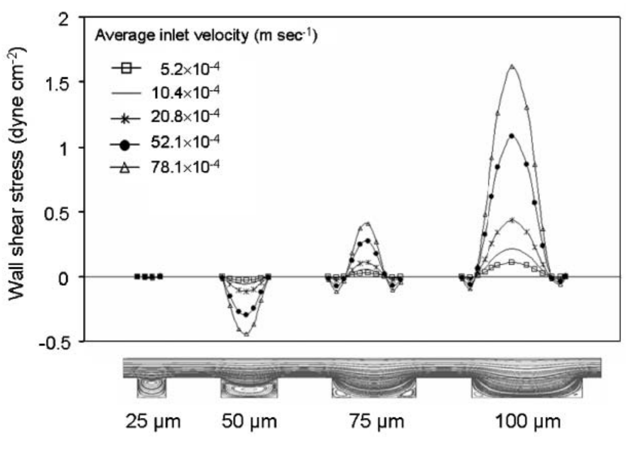
Application: Convective trapping of particles in recirculation regions





J.P. Shelby, D. S.W. Lim, J. S. Kuo, D. T. Chiu, "High radial acceleration in microvortices," Nature, Vol. 425, p.38, 2003

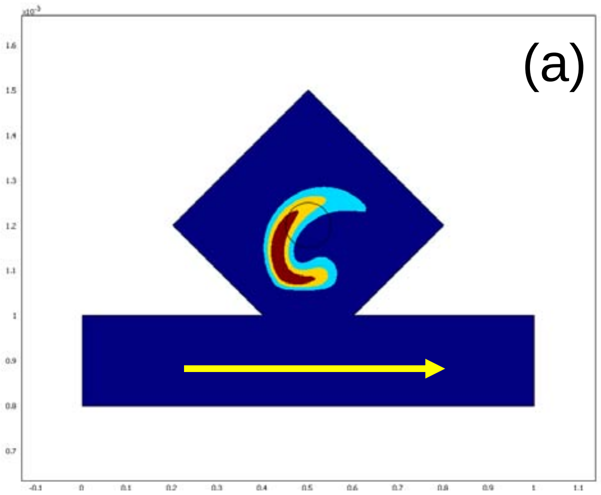


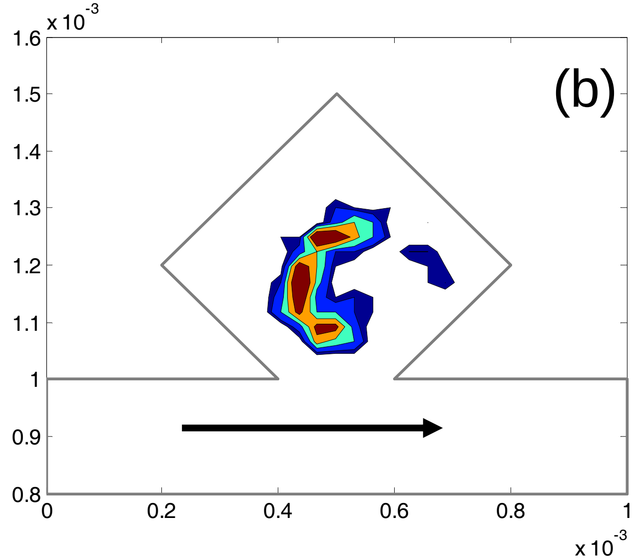


A. Manbachi et al. "Microcirculation within grooved substrates regulates cell positioning and cell docking inside microfluidics channels," Lab chip, ***8****, 747–754, 2008*

Application: Convective trapping of particles in recirculation regions

COMSOL

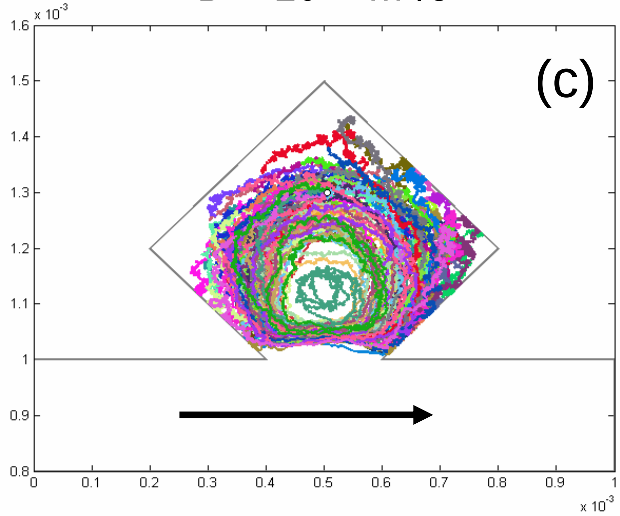




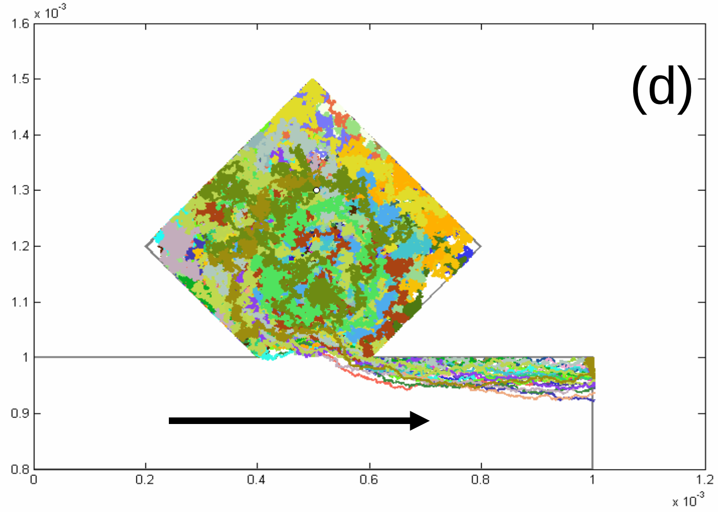
COMSOL / Monte-Carlo

Small diffusion coefficient
$D = 10^{-10}$ m^2/s

Larger diffusion coefficient
$D = 10^{-9}$ m^2/s



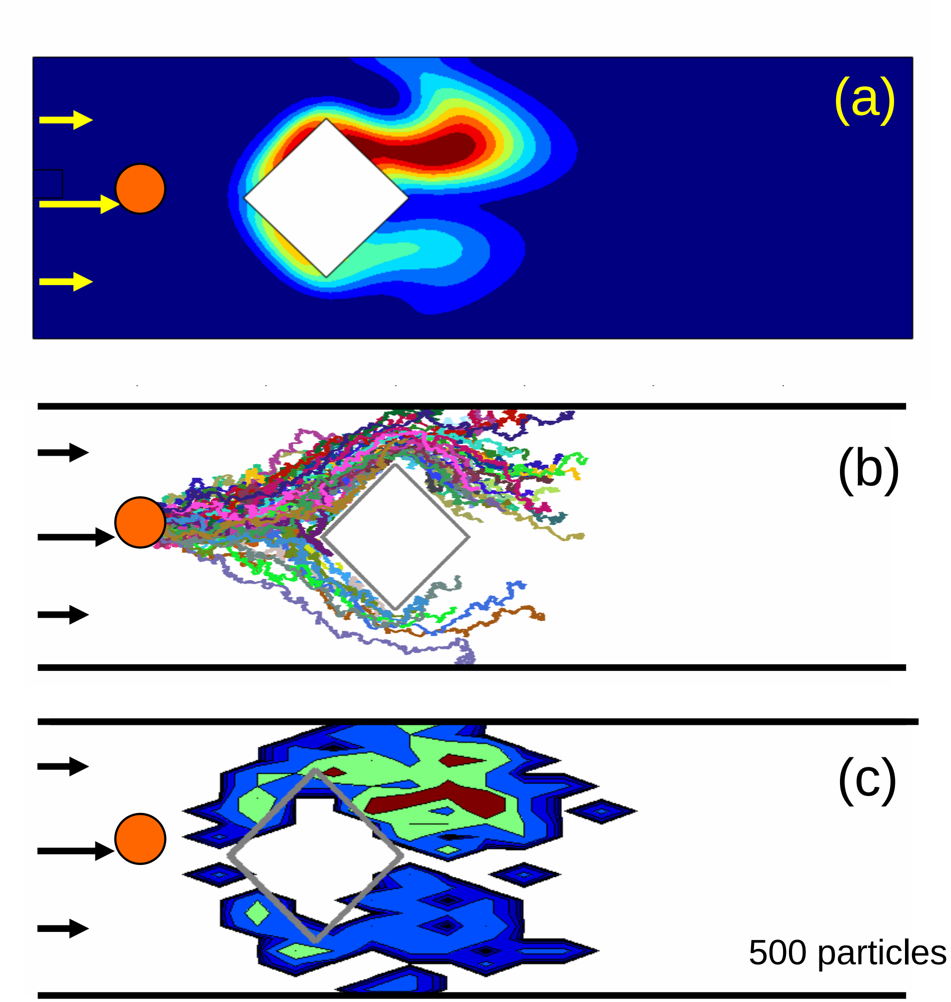
Particles do not escape



Particles slowly escape

Transport of species past a micropillar

- Carrier fluid flow: Poiseuille profile at inlet
- Bolus of concentration released at t=0 from a circular volume above the middle axis

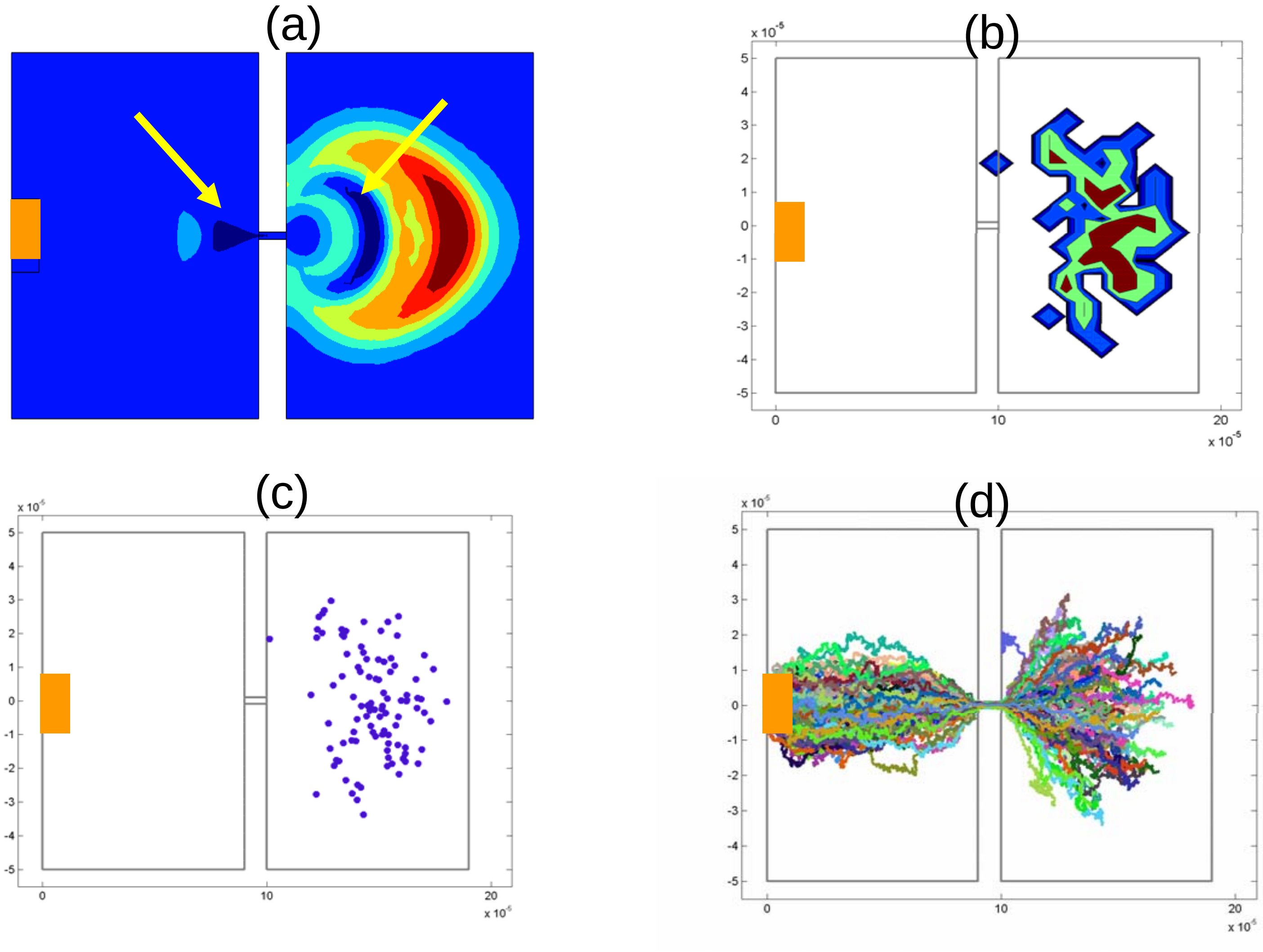


COMSOL

COMSOL / Monte Carlo

Convective diffusion of species / nanoparticles through a micro-hole

- Two chambers separated by a 10 µm aperture
- Bolus of concentration released at t=0 from a rectangular volume



200 particles

3D approach: feasible ?

- Limitation in the number of particles
- Algorithm not complicated
- Geometry and boundaries much more difficult to describe

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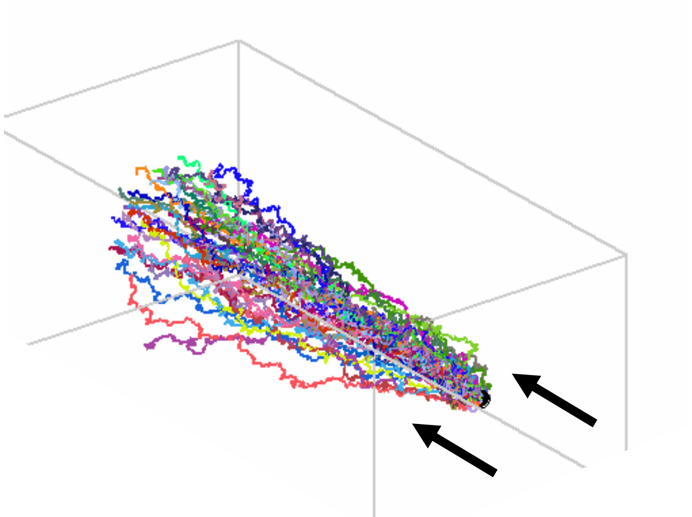
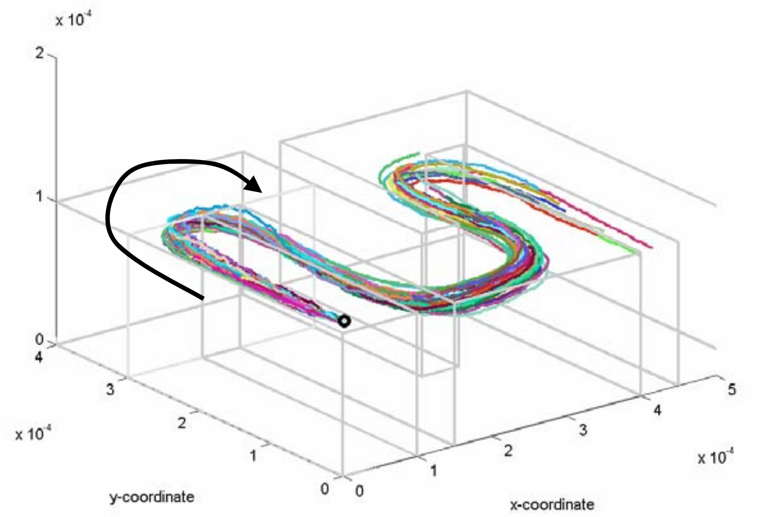
$$Z_{i+1} = Z_i + \sqrt{4\,D\,dt}\,\cos(\beta)$$
$$\alpha = random\ \ (0,2\pi)$$
$$\beta = a\cos\left(1-2\ random(0,1)\right)$$

Convective diffusion from a source point



Convective diffusion in a curved micro-channel

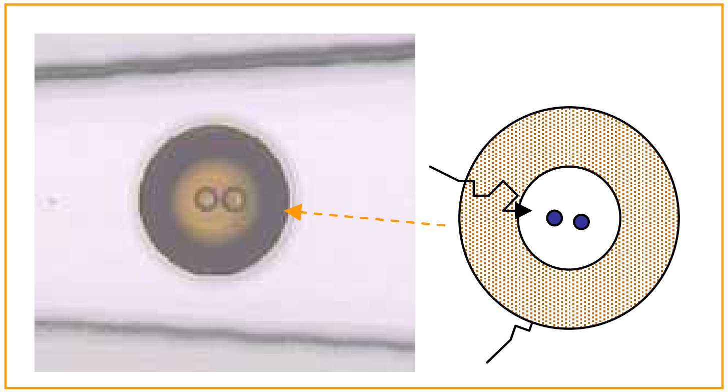


Conclusion / perspectives

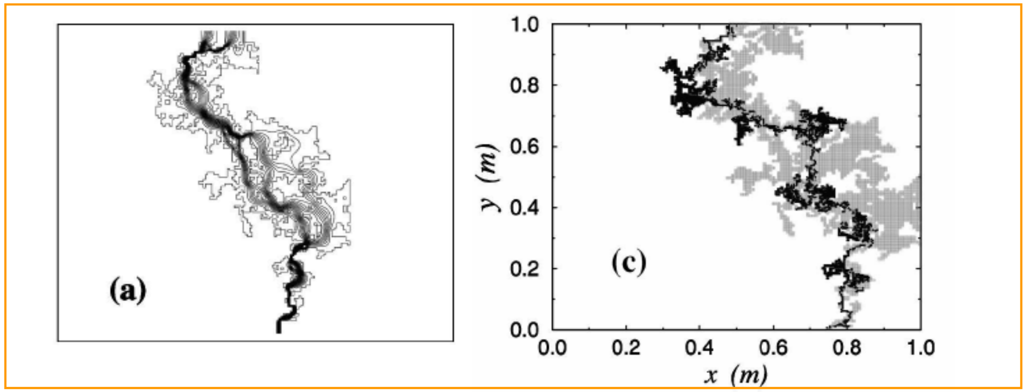
• Continuum method → probability of presence

• COMSOL/ Monte-Carlo interfacing

  - Mimic the transport (to some extend) – visualization tool
  - Avoid numerical problems
  - Easy statistics
  - Necessity for nanopores, nanoporous materials, encapsulation



Le Vot et al. "Non-Newtonian fluids in Flow Focusing Devices: encapsulation with alginates," Proceedings of the 1st European Conference on Microfluidics - Microfluidics 2008 - Bologna, December 10-12, 2008



H.A. Makse et al., "Tracer dispersion in a percolation network with spatial correlations," Physical Review E, Vol 61, n°1, p. 583, 2000

Thanks