Modeling transport in Porous Media: from idealized picture to (real) complex heterogeneous media

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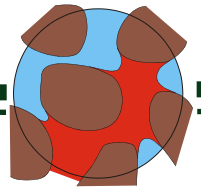
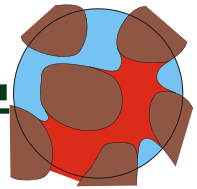
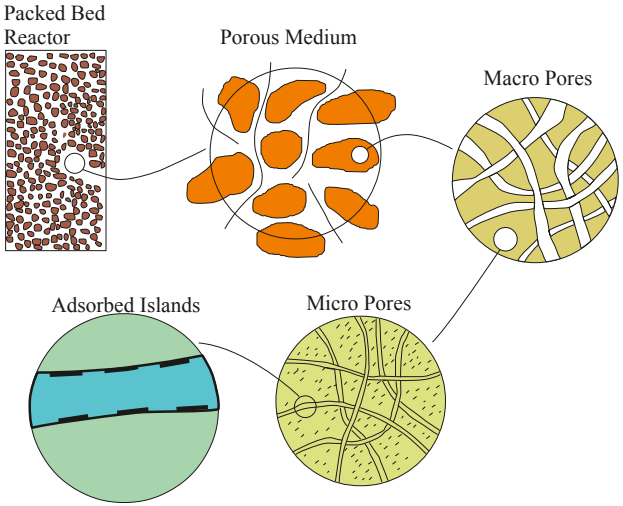


Outline

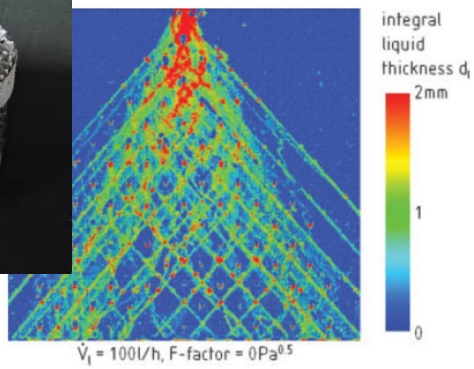
- Introduction
- The idealized picture of multi-scale problems
  - Upscaling techniques
  - Computation of effective properties
- The real world
  - Computation of effective properties on non-periodic images
  - Highly Heterogeneous media:
    - REV or not REV? What is the question?
    - Sequential upscaling
  - Various types of model: N-equations, complex terms (convolution, fractal derivative, etc), hybrid, ...
- Conclusions

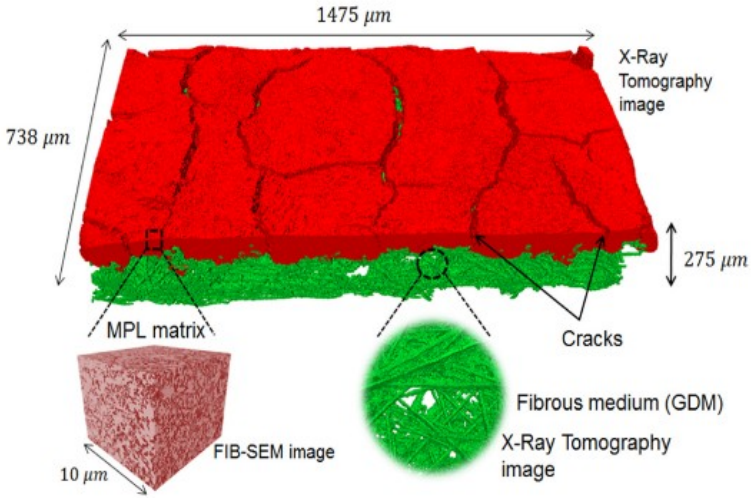


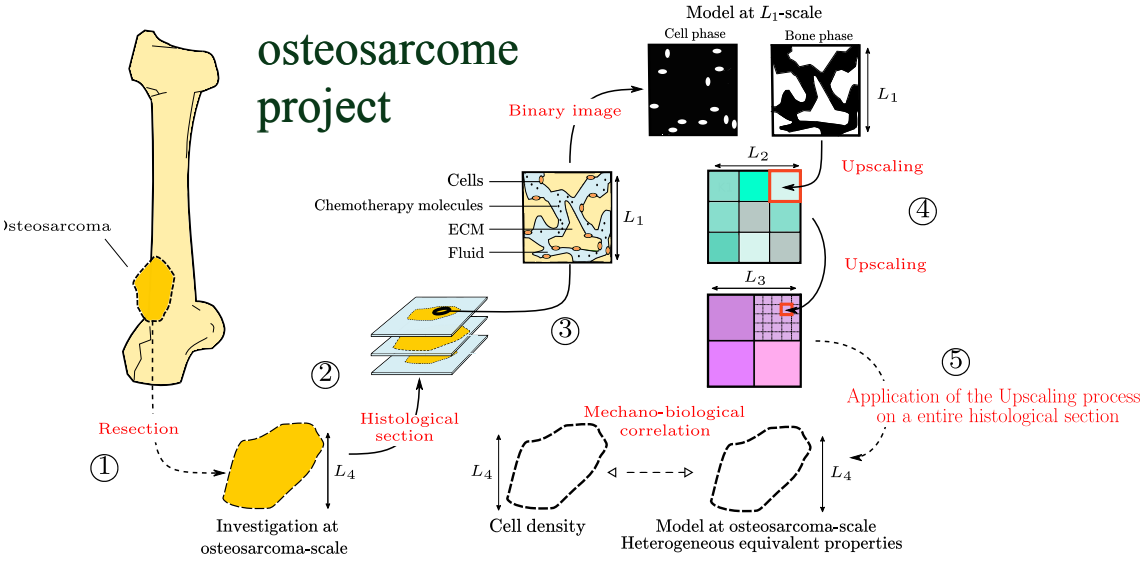
Examples of multi-scale systems

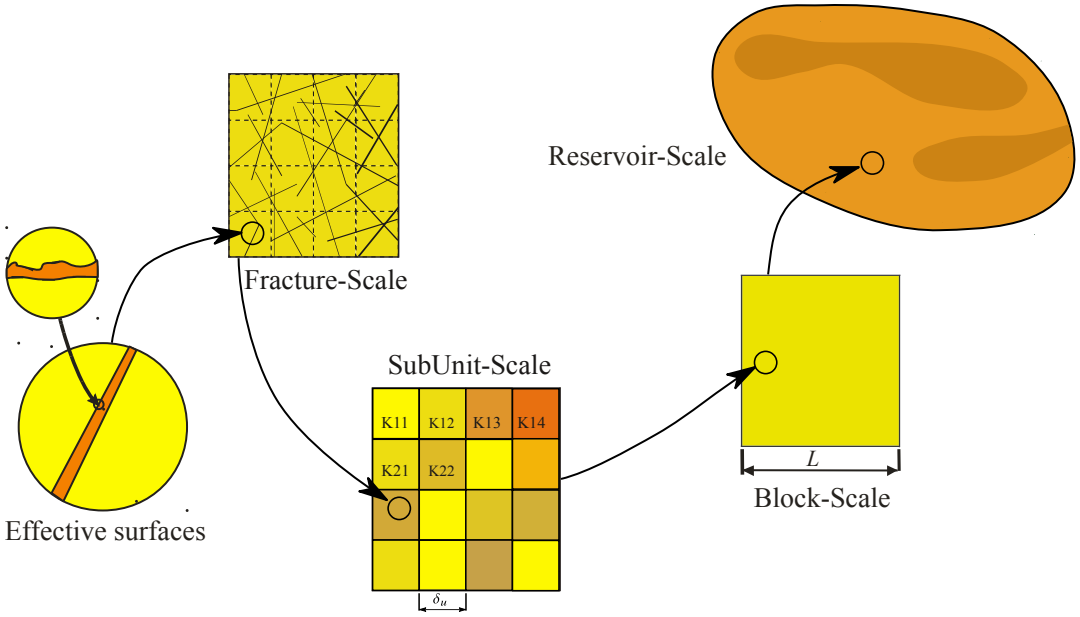


structured media

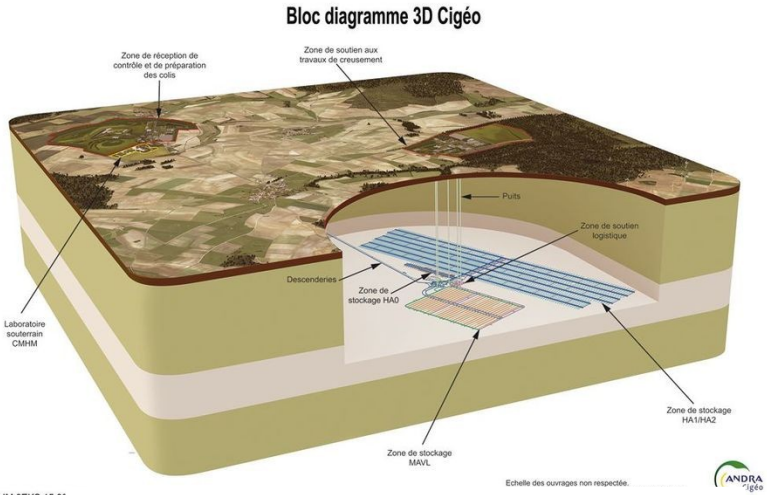




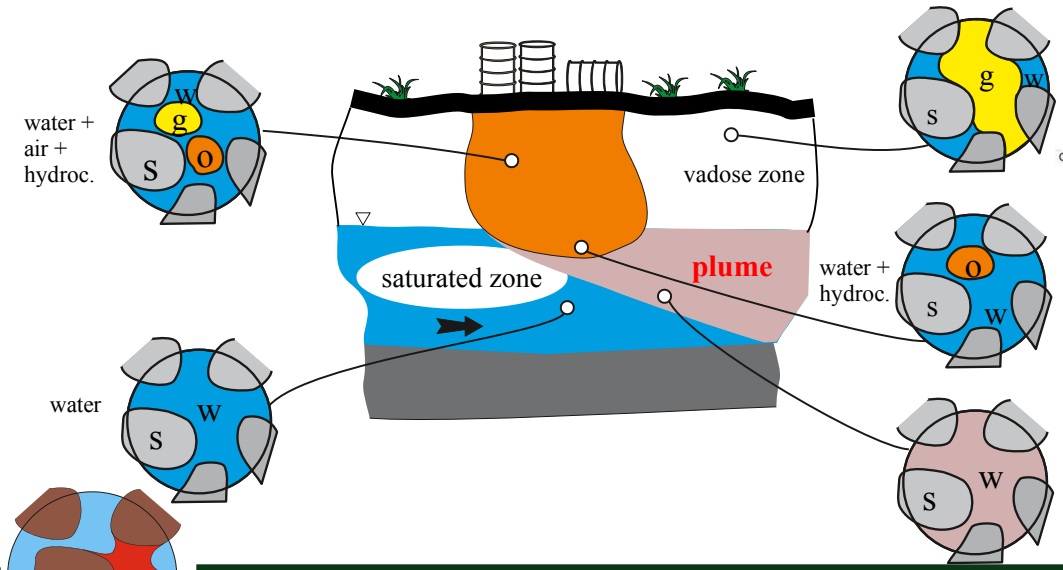




Fractured system

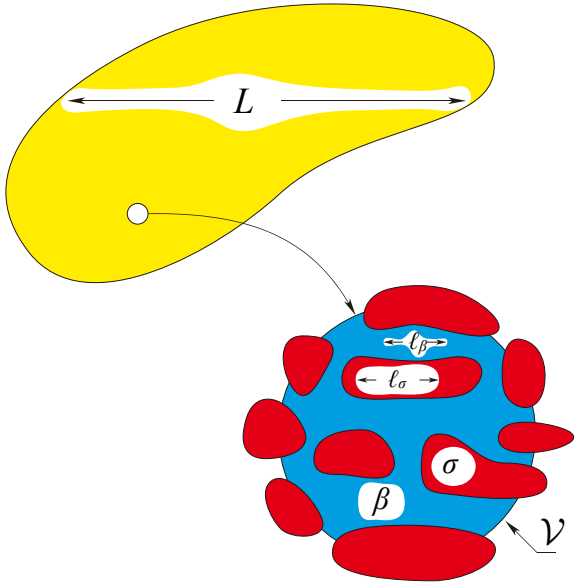


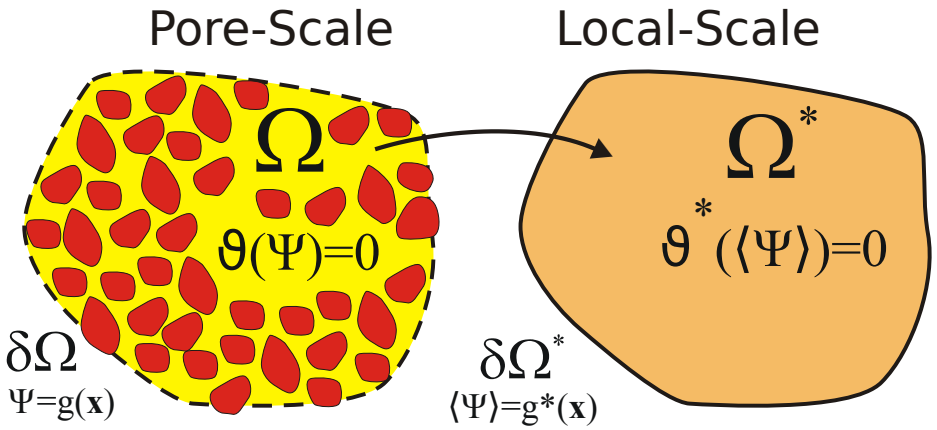
Nuclear Waste storage



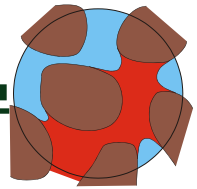
NAPL pollution

Typical (Idealized) Up-Scaling Problem

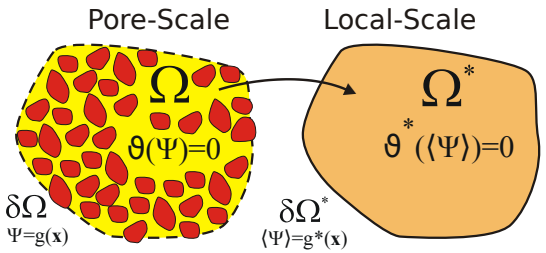




Goal: *method to solve problems with reduced number of DoFs*
Possible route: *obtain macro-scale variables and develop a fully (closed) macro-scale model (equations, effective properties and Bcs)*
Alternative (more accurate?) routes: *hybrid, network, N-equations, etc...*



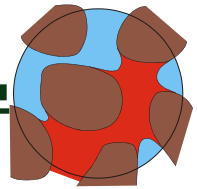
Upscaling: different points of view



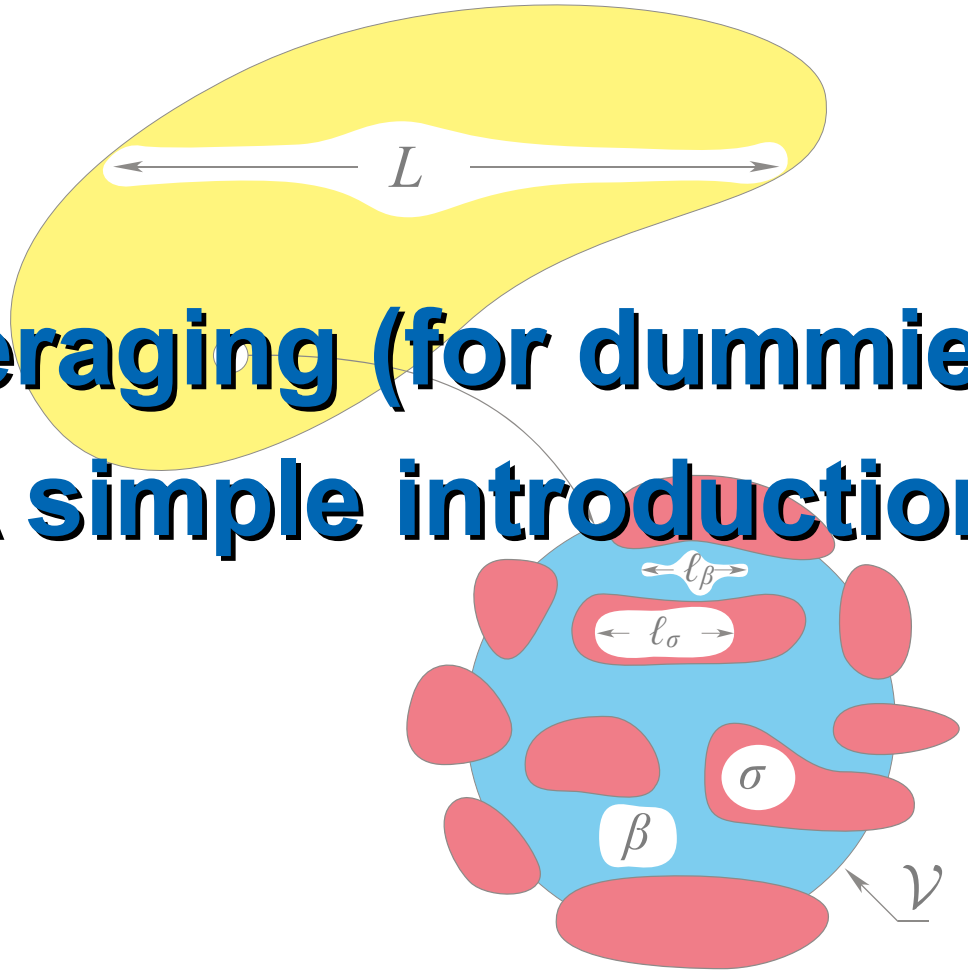
- **Heuristic: Darcy's law (1856)!**
- **Volume averaging + heuristic closure (like CATHARE model)**
- **Volume averaging + irreversible thermodynamics (***Marle, Hassanizadeh, Gray, Bowen (mixture theory), …***)**
- **Upscaling with *closure*: homogenization theory (***Sanchez-Palencia, Bensoussans et al.,...***), volume averaging (***Whitaker, … and variants***),**

$$p_\beta = P_\beta + \tilde{p}_\beta \qquad \tilde{p}_\beta \stackrel{?}{=} f\left(P_\beta, \nabla P_\beta, \ldots\right)$$

- **Stochastic theories (***Matheron, Dagan, Gelhar, ...***), …** $P_\beta = E(p_\beta)$
- **Other point of views...: dual-phase-lagging heat conduction (Wang et al., 2008; Vadasz, 2005...); mixed models; fractional derivatives (Néel,...); CTRW; ...**



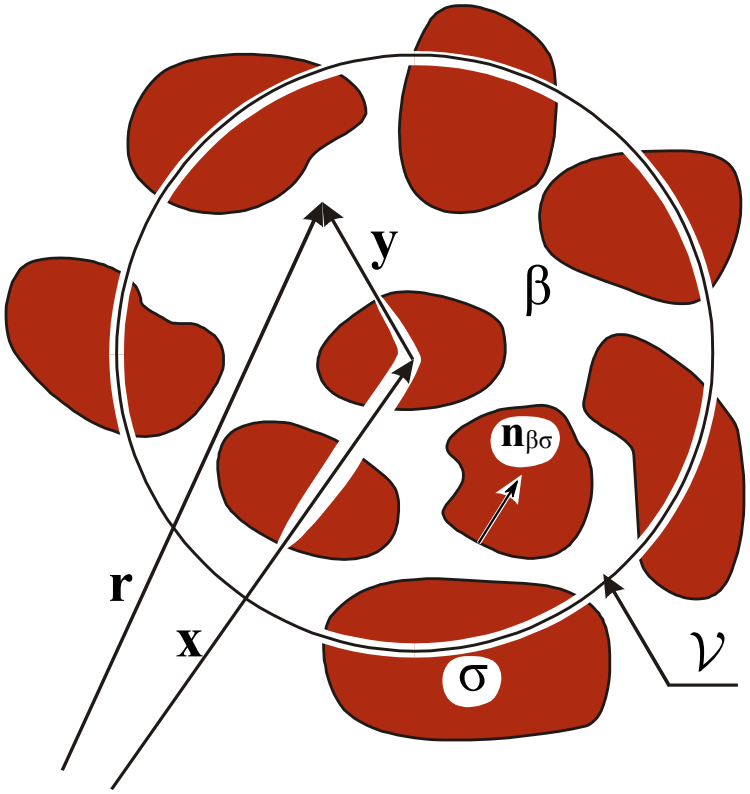
Averaging (for dummies): A simple introduction



see advanced material in Whitaker, The Method of Volume Averaging, 1999

Simple Volume Averaging

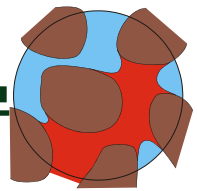
(see early work by Marle, Gray, Whitaker, … in the 60s
see Quintard and Whitaker series on generalized averaging, >93)



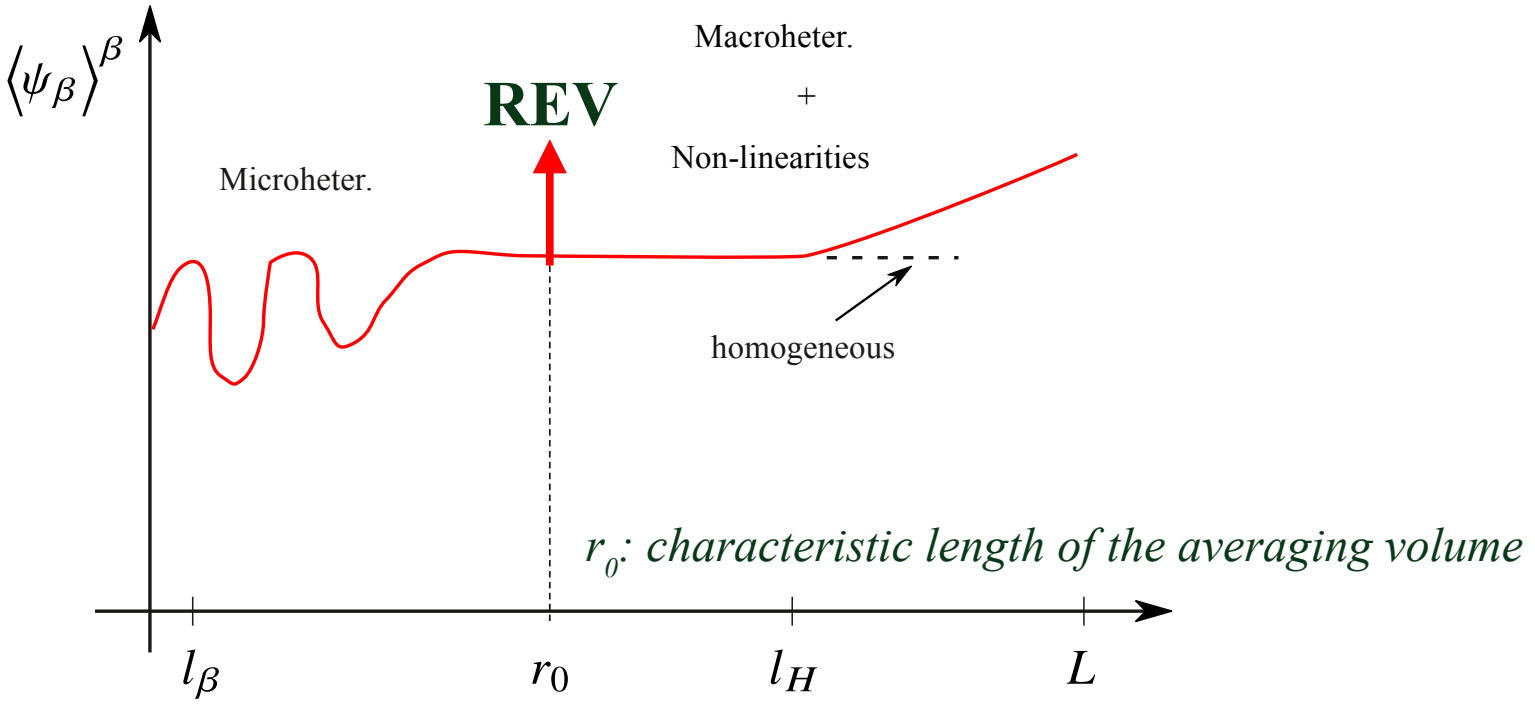
$$\langle \psi_\beta \rangle|_{\mathbf{x}} = \frac{1}{V} \int_{V_\beta} \psi_\beta(\mathbf{x}+\mathbf{y})\, dA$$

- β-phase Volume Fraction $\varepsilon_\beta = \langle \gamma_\beta \rangle$
- β-phase Saturation $\varepsilon_\beta = \varepsilon S_\beta$
- $\langle \psi_\beta \rangle = \varepsilon_\beta \langle \psi_\beta \rangle^\beta$ Intrinsic phase average

Phase indicator: $\gamma_\beta = \begin{cases} 1 & M \in V_\beta \\ 0 & M \notin V_\beta \end{cases}$

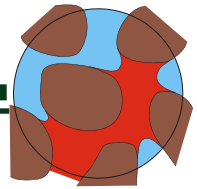


Separation of Scales



If possible, choose: $\ell_\beta << r_0 << l_H << R_0 << L$

If subsequent averaging

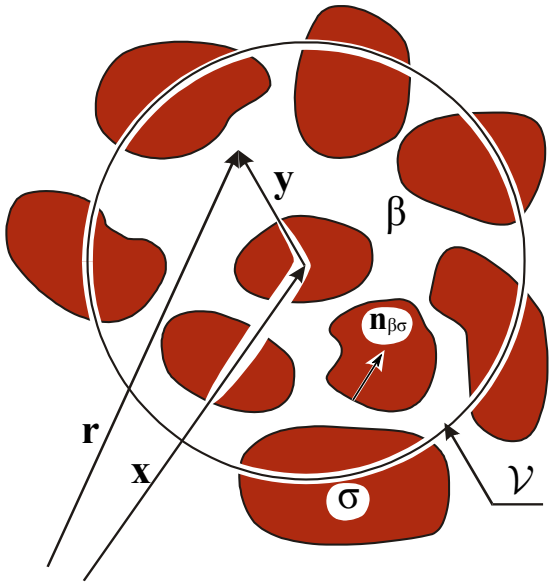


Theorems

$$\left\langle \nabla \psi_\beta \right\rangle = \nabla \left\langle \psi_\beta \right\rangle + \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \psi_\beta \, dA$$

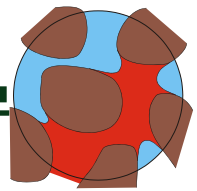
Interfacial Effects (tortuosity,...)

$$\left\langle \nabla \cdot \mathbf{A}_\beta \right\rangle = \nabla \cdot \left\langle \mathbf{A}_\beta \right\rangle + \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \mathbf{A}_\beta \, dA$$



$$\left\langle \frac{\partial \psi_\beta}{\partial t} \right\rangle = \frac{\partial \left\langle \psi_\beta \right\rangle}{\partial t} - \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \mathbf{w}_{\beta\sigma} \psi_\beta \, dA$$

Phase change, dissolution , ...



General structure of a macro-scale equation

- **Pore-scale**

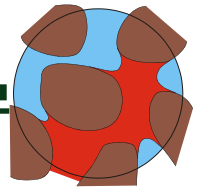
$$\frac{\partial \rho_\beta \omega_\beta}{\partial t} + \nabla . \left(\rho_\beta \omega_\beta \mathbf{v}_\beta \right) = \nabla . \left(\rho_\beta D_\beta \nabla \omega_\beta \right) - \underbrace{r_\beta \left(\omega_\beta \right)}_{\text{homogeneous reaction}}$$

$$\text{B.C. 1} \qquad \mathbf{n}_{\beta\sigma} . \left(\rho_\beta \omega_\beta \left(\mathbf{v}_\beta - \mathbf{w}_{\beta\sigma} \right) - \rho_\beta D_\beta \nabla \omega_\beta \right) = \underbrace{f_\beta \left(\omega_\beta \right)}_{\text{heterogeneous reaction}}$$

- **Macro-scale** **closure?**

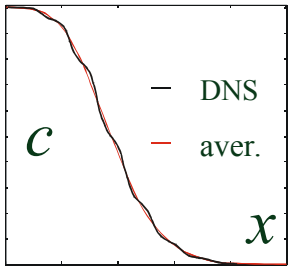
$$\frac{\partial \left\langle \rho_\beta \omega_\beta \right\rangle}{\partial t} + \nabla . \left\langle \rho_\beta \omega_\beta \mathbf{v}_\beta \right\rangle = \nabla . \left(\left\langle \rho_\beta D_\beta \nabla \omega_\beta \right\rangle \right) - \left\langle r_\beta \right\rangle - K_{\beta\sigma}$$

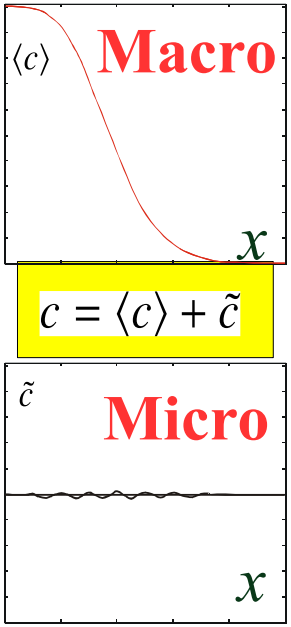
$$\text{with} \quad K_{\beta\sigma} = \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} . \left(\rho_\beta \omega_\beta \left(\mathbf{v}_\beta - \mathbf{w}_{\beta\sigma} \right) - \rho_\beta D_\beta \nabla \omega_\beta \right) dA$$



Upscaling with *closure*: a schematic view for diffusion in a heterogeneous medium

$$\frac{\partial c}{\partial t} = \nabla.(\mathbf{k}(x).\nabla c)$$



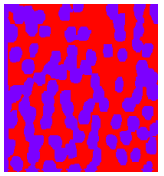


$$\frac{\partial \langle c \rangle}{\partial t} = \nabla.\langle \mathbf{k}(\mathbf{x}).\nabla(\langle c \rangle + \tilde{c}) \rangle$$

Closure:

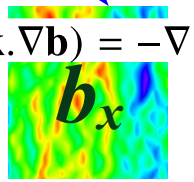
$$\tilde{c} = \mathbf{b}.\nabla\langle c \rangle + O(\ell^2/L^2)$$

$$\frac{\partial \tilde{c}}{\partial t} = \nabla.(\mathbf{k}.\nabla\tilde{c}) + \nabla.(\tilde{\mathbf{k}}.\nabla\langle c \rangle) - \nabla.\langle \mathbf{k}.\nabla\tilde{c} \rangle$$



- Tomography
- Reconstruction
- Geostatistics
- ...

$$\nabla \cdot (\mathbf{k}.\nabla\mathbf{b}) = -\nabla \cdot \tilde{\mathbf{k}}$$



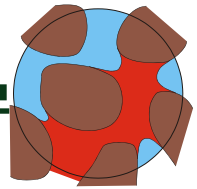
Macro-scale Equation

$$\frac{\partial \langle c \rangle}{\partial t} = \nabla.(\mathbf{K}_{eff}.\nabla\langle c \rangle)$$

Effective Properties

$$\mathbf{K}_{eff} = \langle \mathbf{k} \rangle + \langle \mathbf{k}.\nabla\mathbf{b} \rangle$$

Note: High Performance Computing → up to 2048^3 voxels



Closure and Macro-scale equation : effective diffusion

$$\tilde{c}_\beta = \mathbf{b}_\beta . \nabla C_\beta + \ldots \qquad C_\beta = \langle c_\beta \rangle^\beta$$

- Local problem over *representative* UC

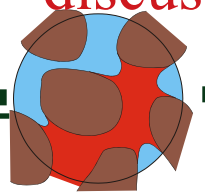
$$0 = \nabla^2 \mathbf{b}_\beta$$

B.C. 1 $\quad \mathbf{n}_{\beta\sigma} \cdot \nabla \mathbf{b}_\beta = -\mathbf{n}_{\beta\sigma}$ at $A_{\beta\sigma}$

$$\mathbf{b}_\beta(\mathbf{r}) = \mathbf{b}_\beta(\mathbf{r} + \mathbf{l}_i)$$

$$\langle \mathbf{b}_\beta \rangle^\beta = 0$$

Periodicity? To be discussed!



- Macro-scale Equation

$$\frac{\partial \varepsilon_\beta C_\beta}{\partial t} = \nabla . \left(\varepsilon_\beta \mathbf{D}^*_\beta \cdot \nabla C_\beta \right)$$

$$\mathbf{J}^*_\beta = -\varepsilon_\beta \mathbf{D}^*_\beta \cdot \nabla C_\beta$$

macro-scale flux density

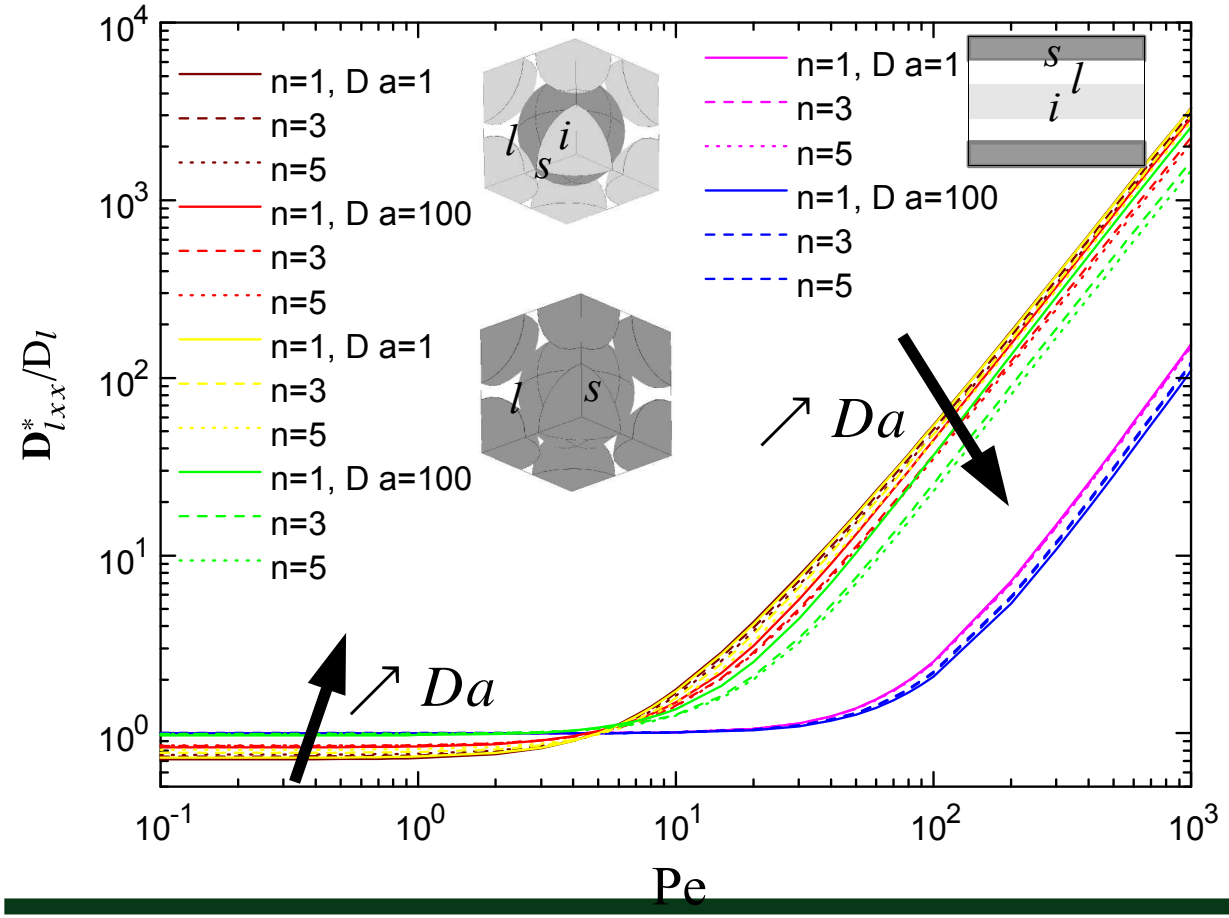
- **Effective diffusion tensor**

$$\mathbf{D}^*_\beta = D_\beta \left(\mathbf{I} + \frac{1}{\mathcal{V}_\beta} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \mathbf{b}_\beta \, dA \right)$$

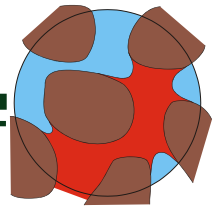
If isotropic: $\mathbf{D}^*_\beta = \dfrac{D_\beta}{\tau_\beta} \mathbf{I}$ tortuosity: $\tau_\beta \geq 1$

Example: Dispersion with heterogeneous reaction

Da=0 → passive case ; Da → ∞ → uniform conc. at A_{ls}

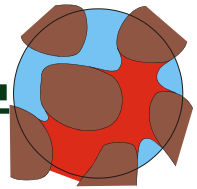


Guo et al., 2015

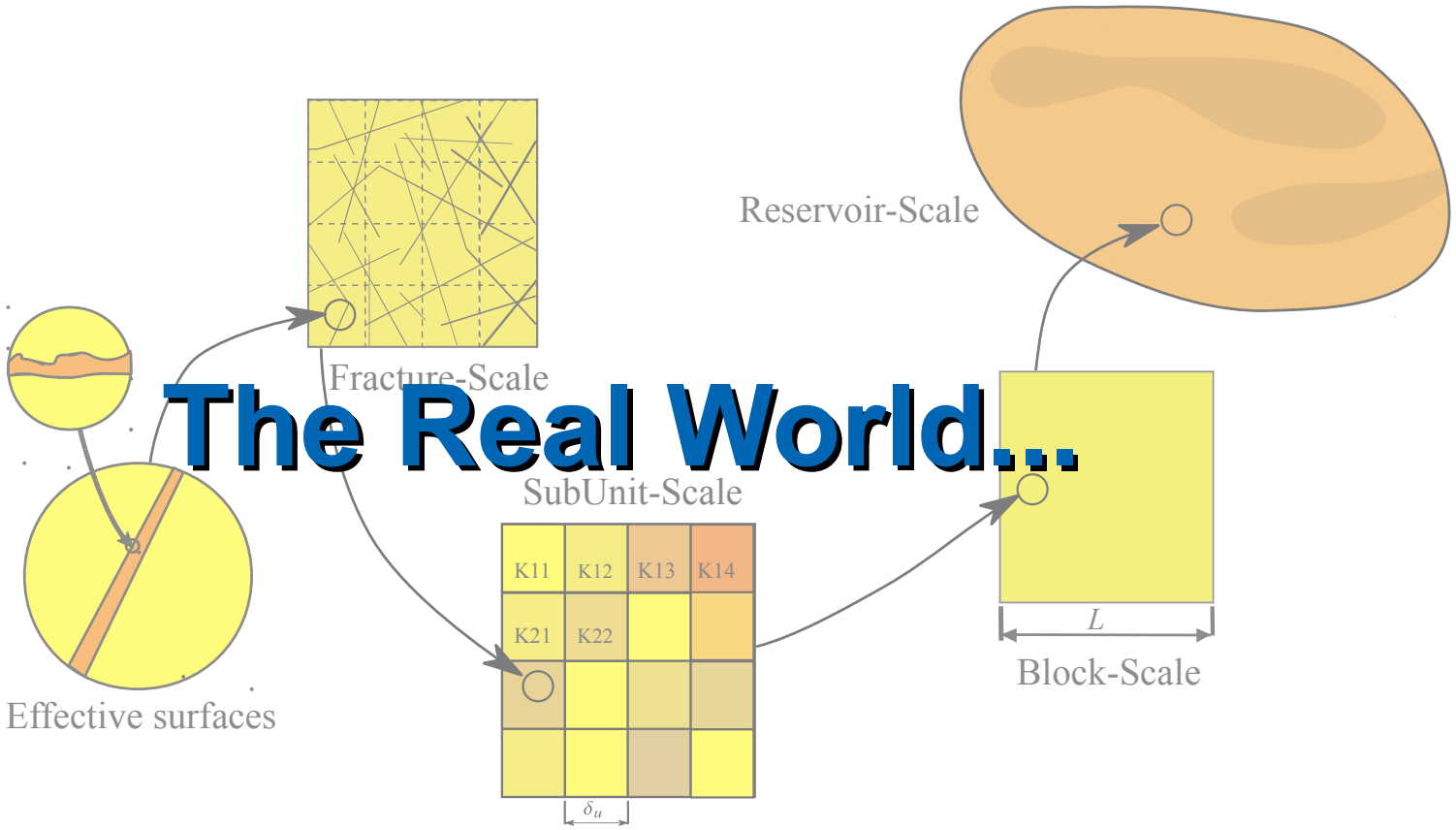


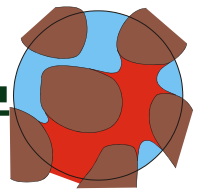
Conclusions and problems

- Upscaling gives insight into appropriate equations and effective properties
- Attractive framework for modeling and working with pore-scale images combining imaging/upscaling/HPC
- ...BUT, in the REAL WORLD:
  - Non-periodic cases
  - Bad or no separation of scales
  - Non-local terms in space and time
  - Non-linear and coupled transport problems (e.g. no linear closure)
  - Effective Boundary conditions



The Real World...





Eff. Prop. for Non-Periodic Images

Case of "diffusion" problems: e.g., permeability, effective diffusion

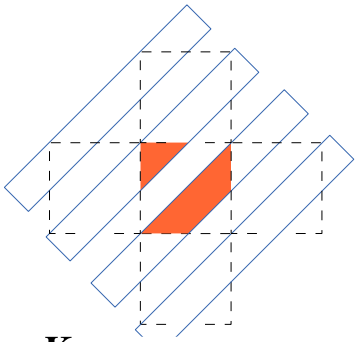
- **Periodicity : natural handling of anisotropy effects**
- **Making image periodic?**

See discussion in Guibert et al., 2015

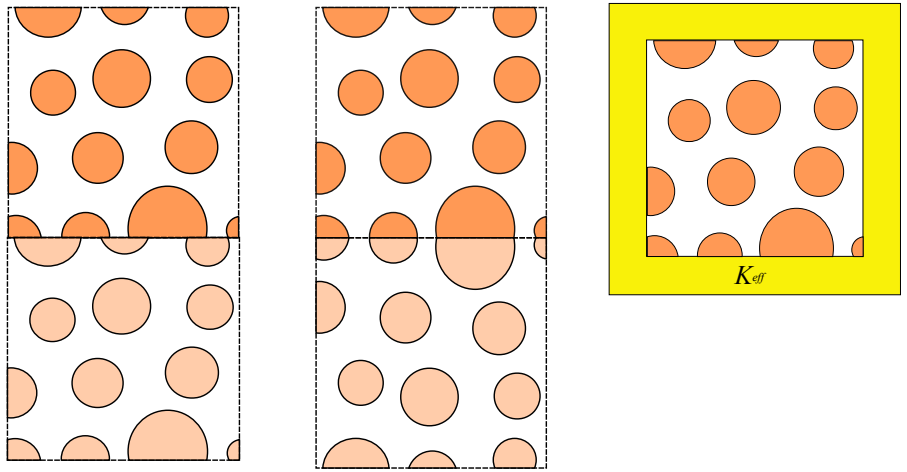
I: Percolation problem

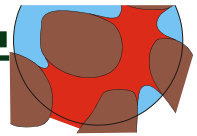
II: Loss of anisotropy features

III: potentially various biases



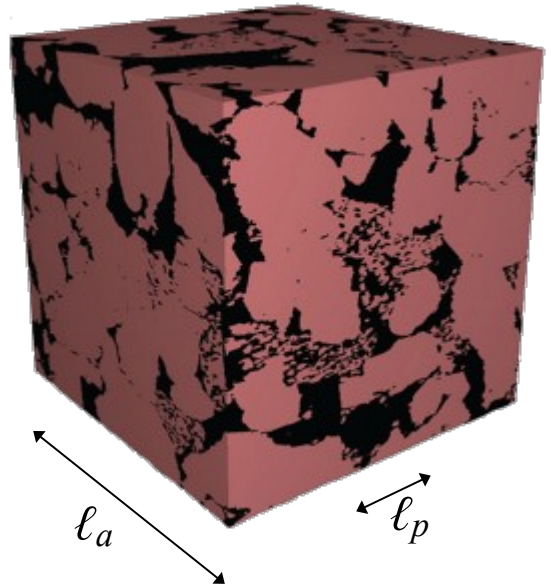
$$\mathbf{K}_{eff} = \varepsilon_\beta \mathbf{K}_\beta + \varepsilon_\sigma \mathbf{K}_\sigma + \frac{\varepsilon_\beta \varepsilon_\sigma \left(\mathbf{K}_\beta - \mathbf{K}_\sigma\right) \cdot \mathbf{ii} \cdot \left(\mathbf{K}_\sigma - \mathbf{K}_\beta\right)}{\mathbf{i} \cdot \left(\varepsilon_\beta \mathbf{K}_\sigma + \varepsilon_\sigma \mathbf{K}_\beta\right) \cdot \mathbf{i}}$$





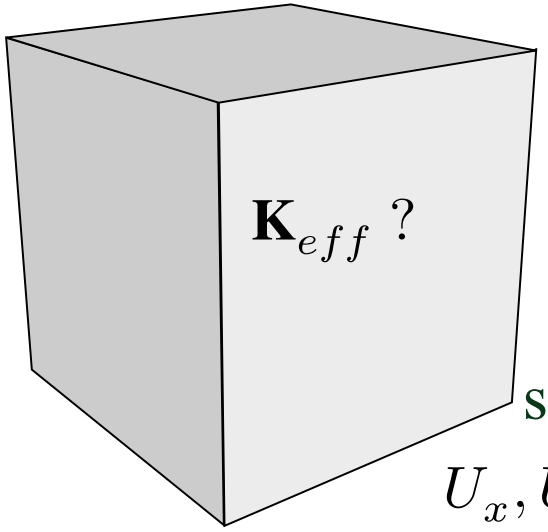
Calculations over non-periodic images (cont.): "permeameters"

Small-scale



solve for
v_x, v_y, v_z, p

Macro-scale



solve for
U_x, U_y, U_z, P

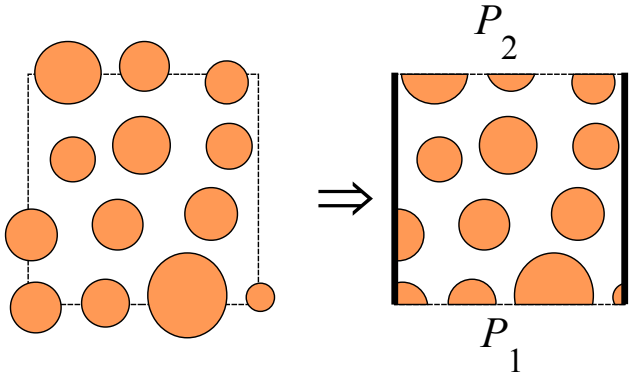
Equivalence: determine $\mathbf{K}_{eff}$ to satisfy

$$\langle U_x \rangle = \langle v_x \rangle \ , \ \langle U_y \rangle = \langle v_y \rangle \ , \ \langle U_z \rangle = \langle v_z \rangle$$

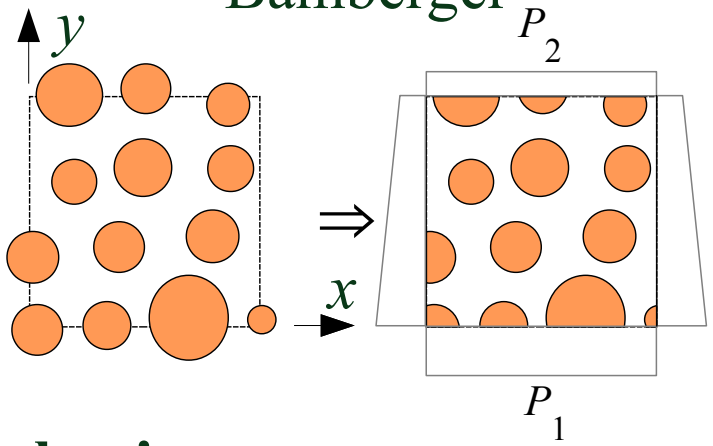
See discussion in: Manwart et al. 2002; Piller et al. 2009; Guibert et al., 2015; ...

Choice of Boundary Conditions

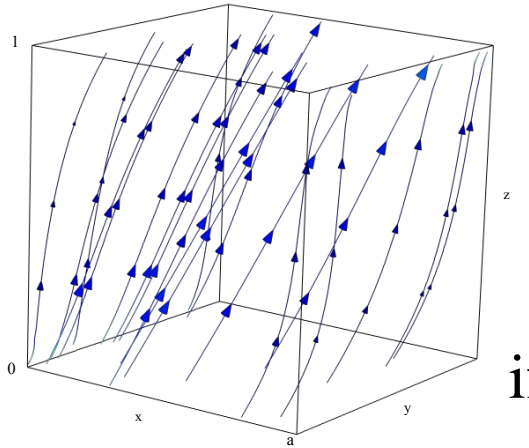
Classical



Bamberger



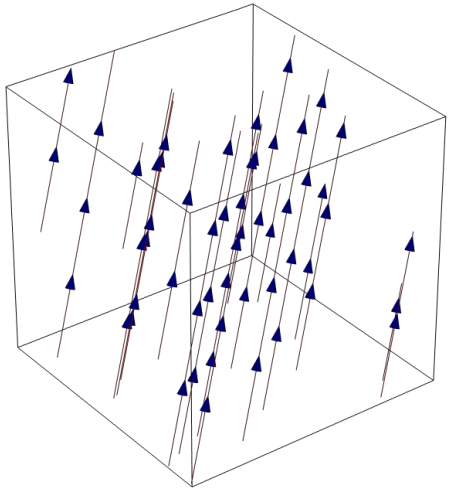
if homogeneous box!

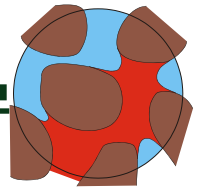


$$\text{if } \frac{\ell_a}{\ell_H} \to \infty \quad \to$$

infinite layer
1D anal. sol.

$=$





Interpretation

1) Optimization (whatever the technique): vary $\mathbf{K}_{eff}$ to satisfy

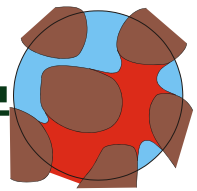
$$\langle U_x \rangle = \langle v_x \rangle \ , \ \langle U_y \rangle = \langle v_y \rangle \ , \ \langle U_z \rangle = \langle v_z \rangle$$

2) Approximation: Assume 1D infinite layer

$\langle U_i \rangle = U_i$ (1D infinite layer), therefore (case $\nabla P = -\frac{P_1 - P_2}{\ell_H}\mathbf{e}_x$):

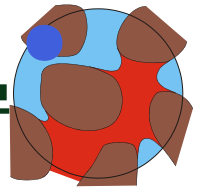
$$\langle v_x \rangle = K_{xx}\frac{1}{\mu}\frac{P_1 - P_2}{\ell_H} \ ; \ \langle v_y \rangle = K_{yx}\frac{1}{\mu}\frac{P_1 - P_2}{\ell_H} \ ; \ \langle v_z \rangle = K_{zx}\frac{1}{\mu}\frac{P_1 - P_2}{\ell_H}$$

$\rightarrow$ complete determination of $\mathbf{K}_{eff}$ through 3 calculations, changing the orientation of the averaged gradient



Discussion

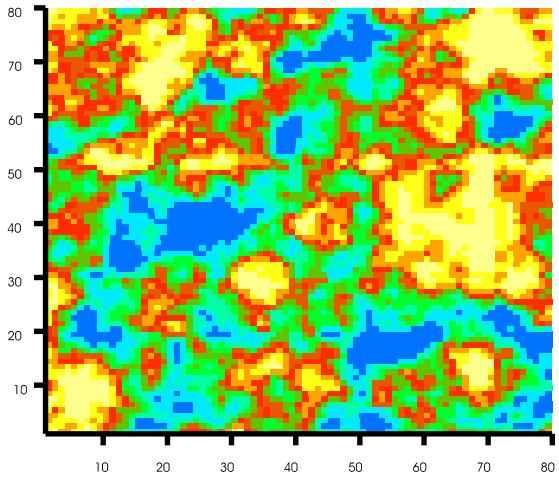
- Biases due to ℓ_p/ℓ_H and ℓ_a/ℓ_H
- Symmetry of the Effective tensor:
  - case of periodic conditions: leads naturally to a symmetrical $\mathbf{K}_{eff}$
  - Technique 1: symmetry of $\mathbf{K}_{eff}$ can be imposed
  - Technique 2: symmetry is not enforced
    - can be used as it is, but no principle axis (see Zijl, Wouter, "The symmetry approximation for nonsymmetric permeability tensors and its consequences for mass transport", Transport in Porous Media 22, 2 (1996), pp. 121–136.)
    - or use $\frac{1}{2}\left(\mathbf{K}_{eff} + \mathbf{K}_{eff}^T\right)$

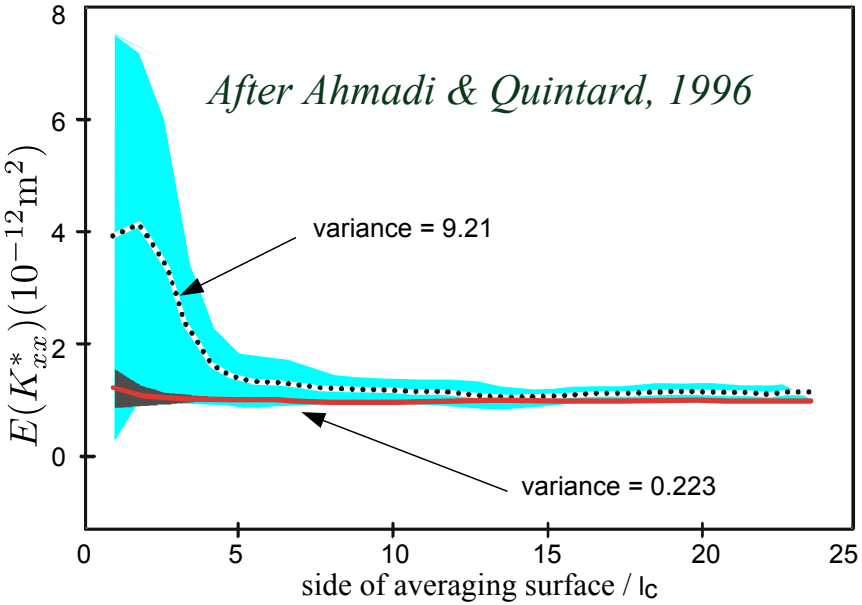


Example 1: large-scale permeability

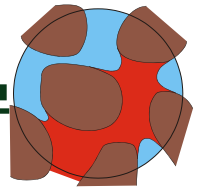
k(**x**): Lognormal distribution, spatial correlation length ℓ_c

$$\mathbf{K}_{eff} = \langle \mathbf{k} \rangle + \langle \mathbf{k}.\nabla \mathbf{b} \rangle$$

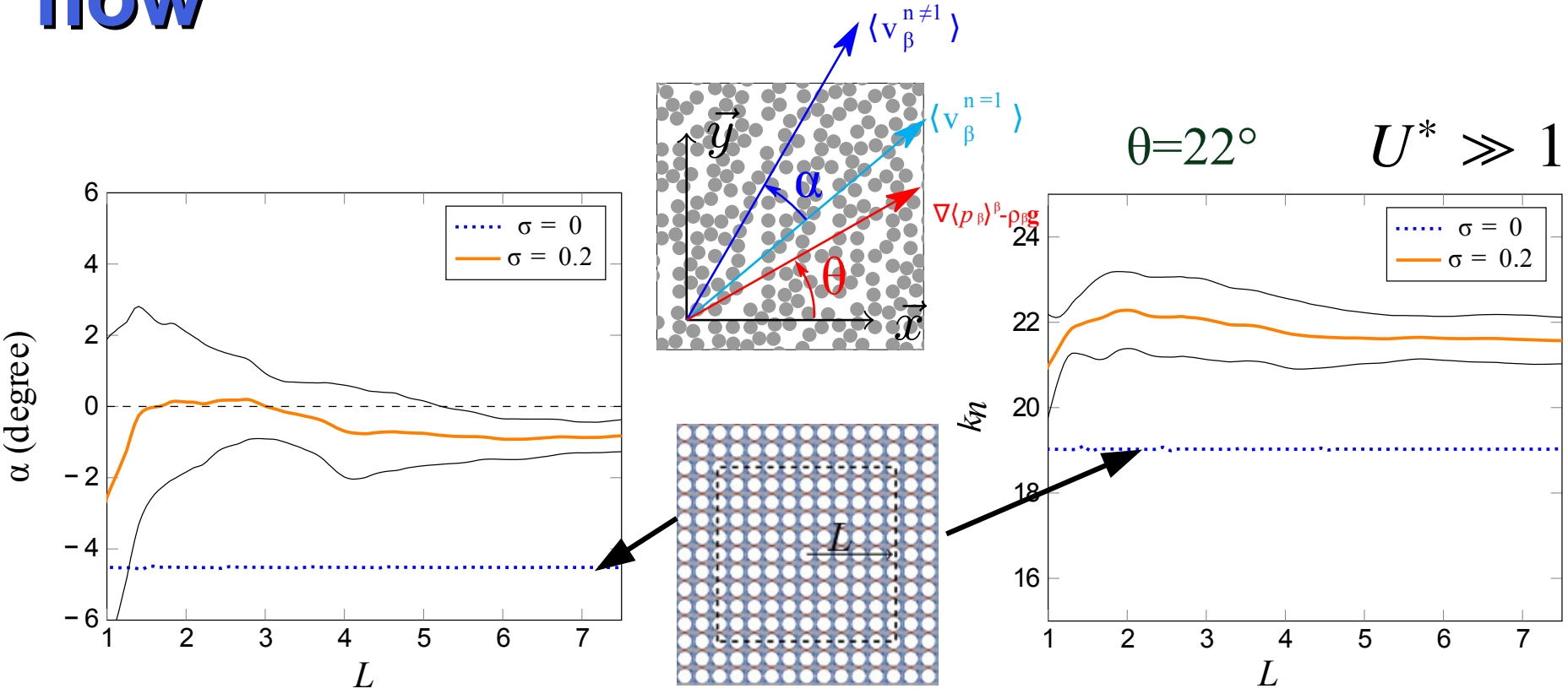




note that it may be difficult in practice to satisfy a REV condition!



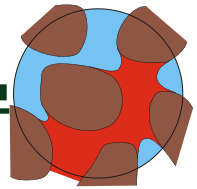
Example 2: non-newtonian fluid flow



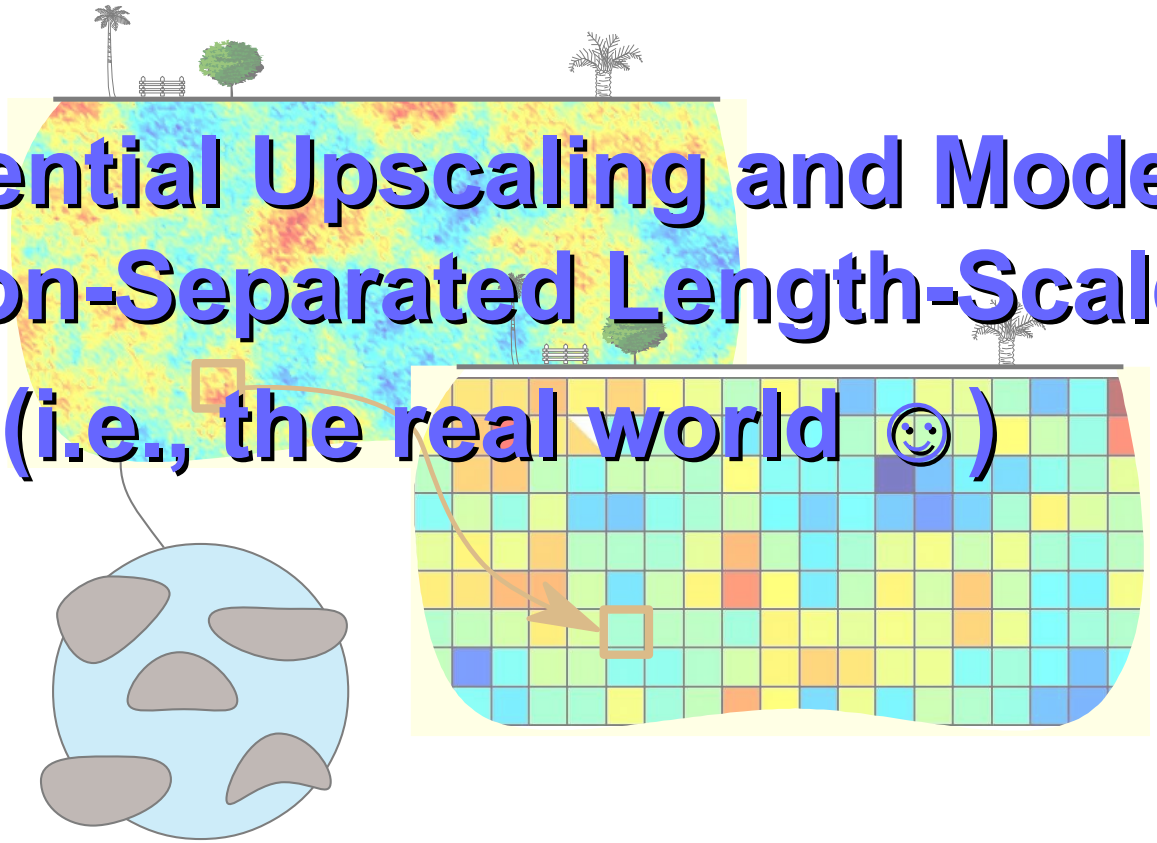
Flow of a non-newtonian fluid (from Zami-Pierre et al., 2018)

Beyond REV paradigm

- Interest of having a REV:
  - convergence properties with ℓ_{REV}/L
  - above ℓ_{REV}, same equation structure and effective properties
  - calculation over *one sample* gives a good estimate of transport properties
- Note that this is not a purely geometric notion (it is process dependent)
- What to do, if no REV properties!

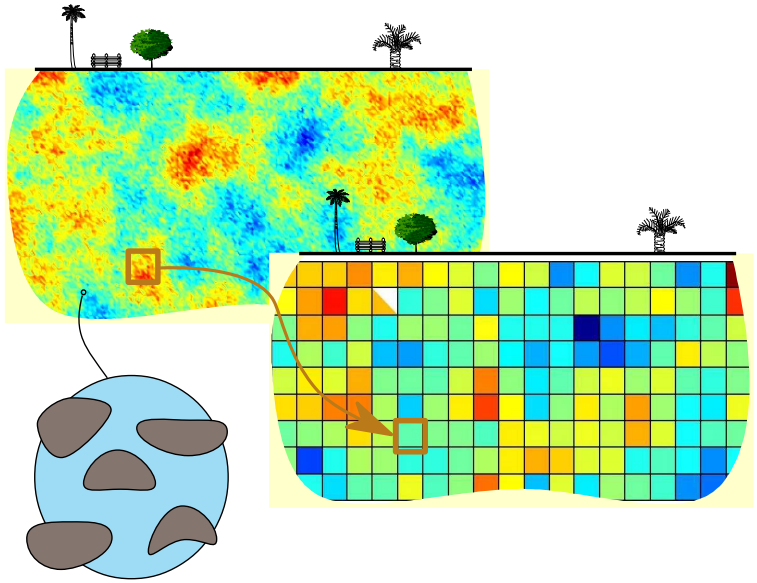


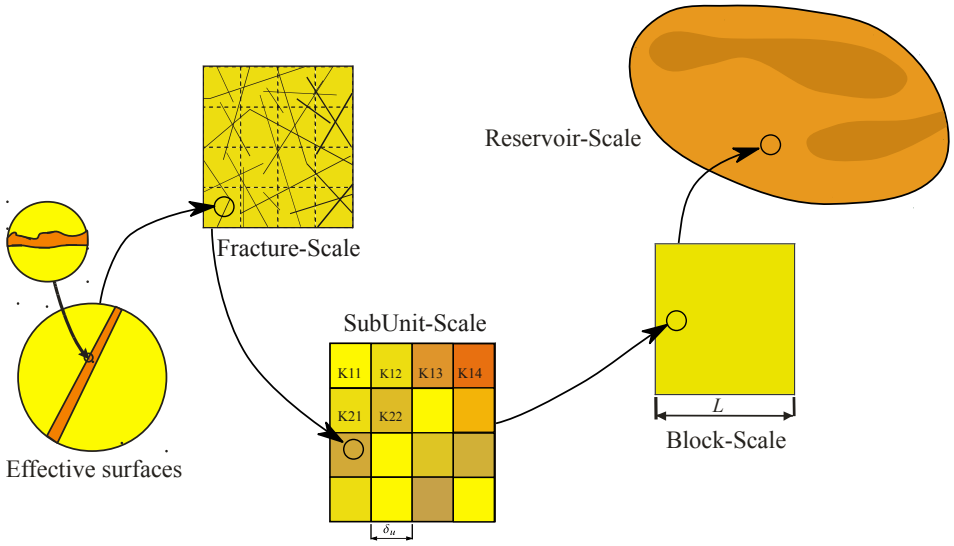
Sequential Upscaling and Models for Non-Separated Length-Scales (i.e., the real world ☺)



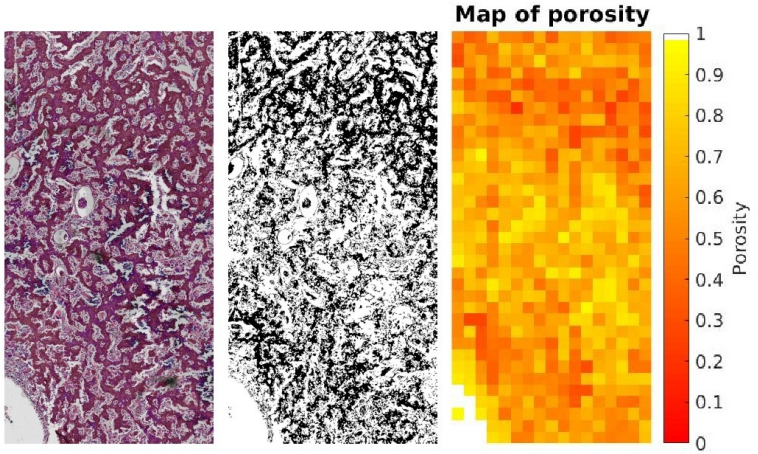
Examples

Pet. Engng, Hydrogeology



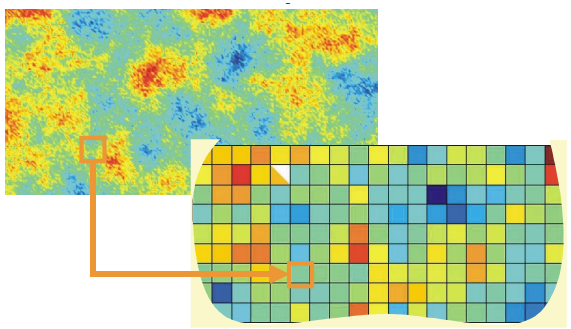


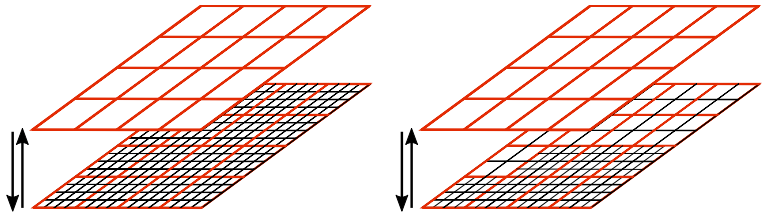
Pauline Assemat project
on osteosarcoma



Sequential upscaling as a tool for GridBlock aggregation, multigrid or AMR algorithms

- GridBlock models: no separation of scales



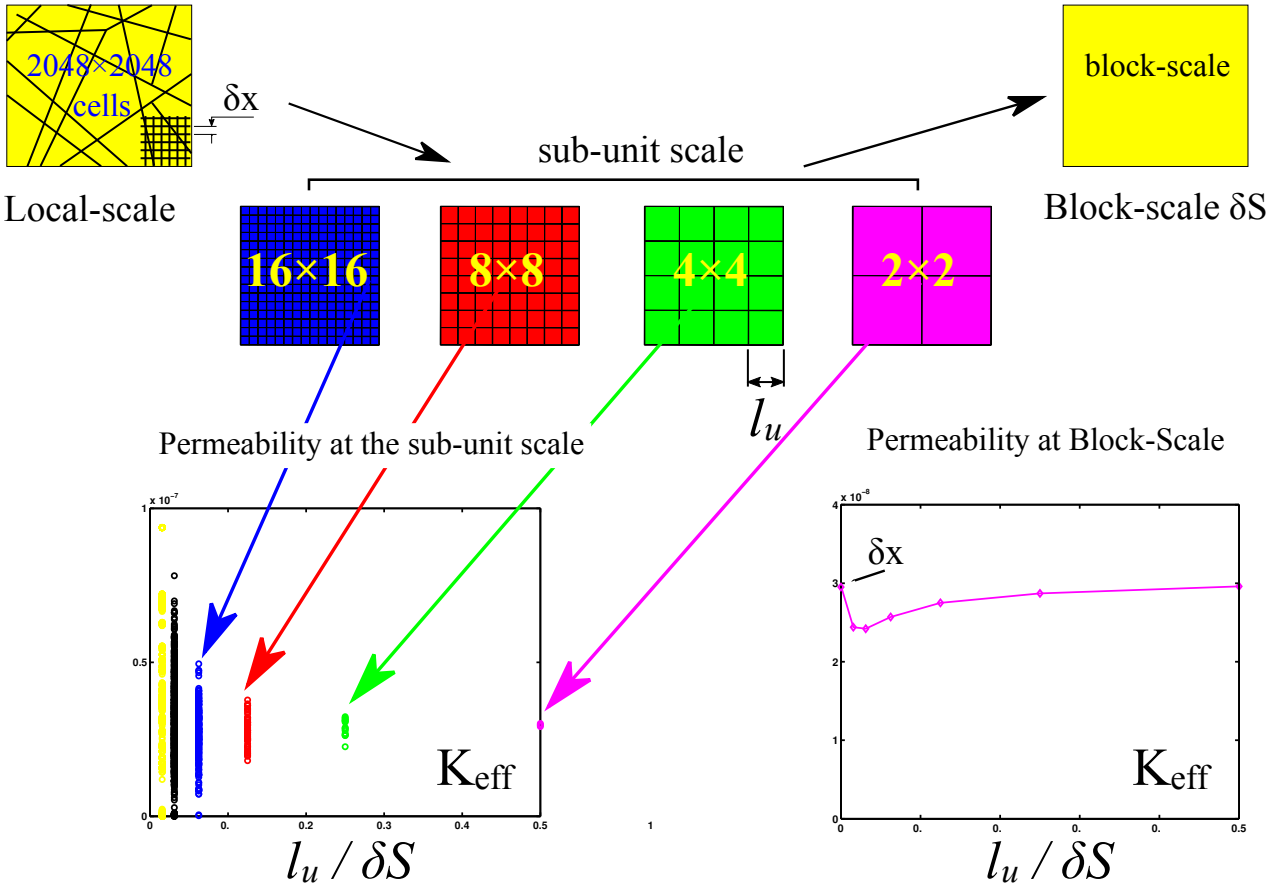


- Multigrid, AMR: need projection operators taking into account heterogeneity effects!

assumption of a constant form of the transport equations at all levels!

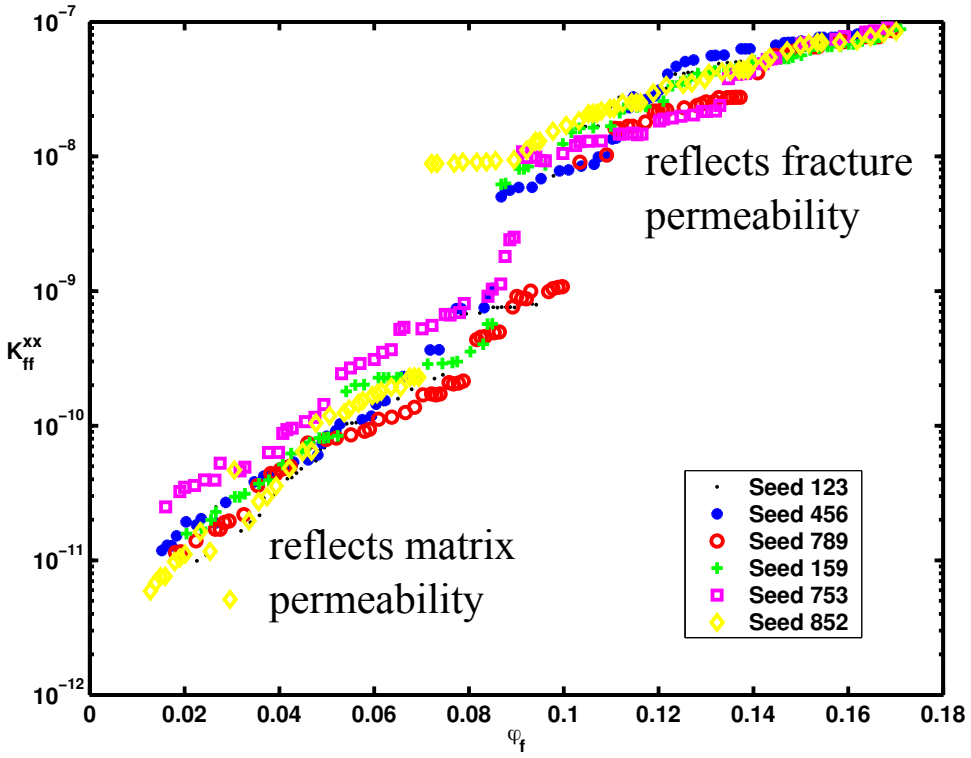
2-step sequential: ex. of a Fractured system

from Kfoury et al., 2004, 2006, ...

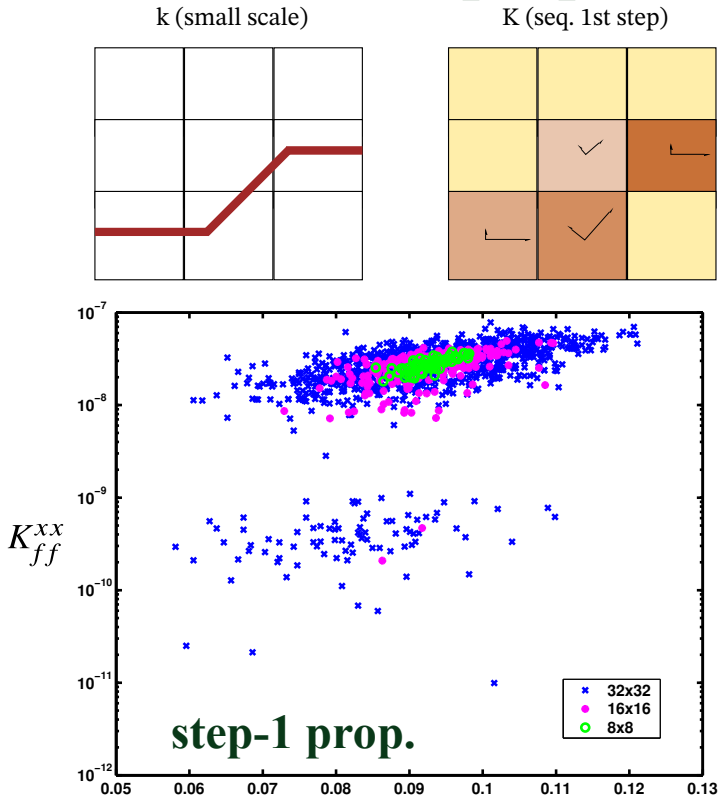


Example: also approximates percolation properties

from Kfoury et al., 2004, 2006, ...



Percolation properties?

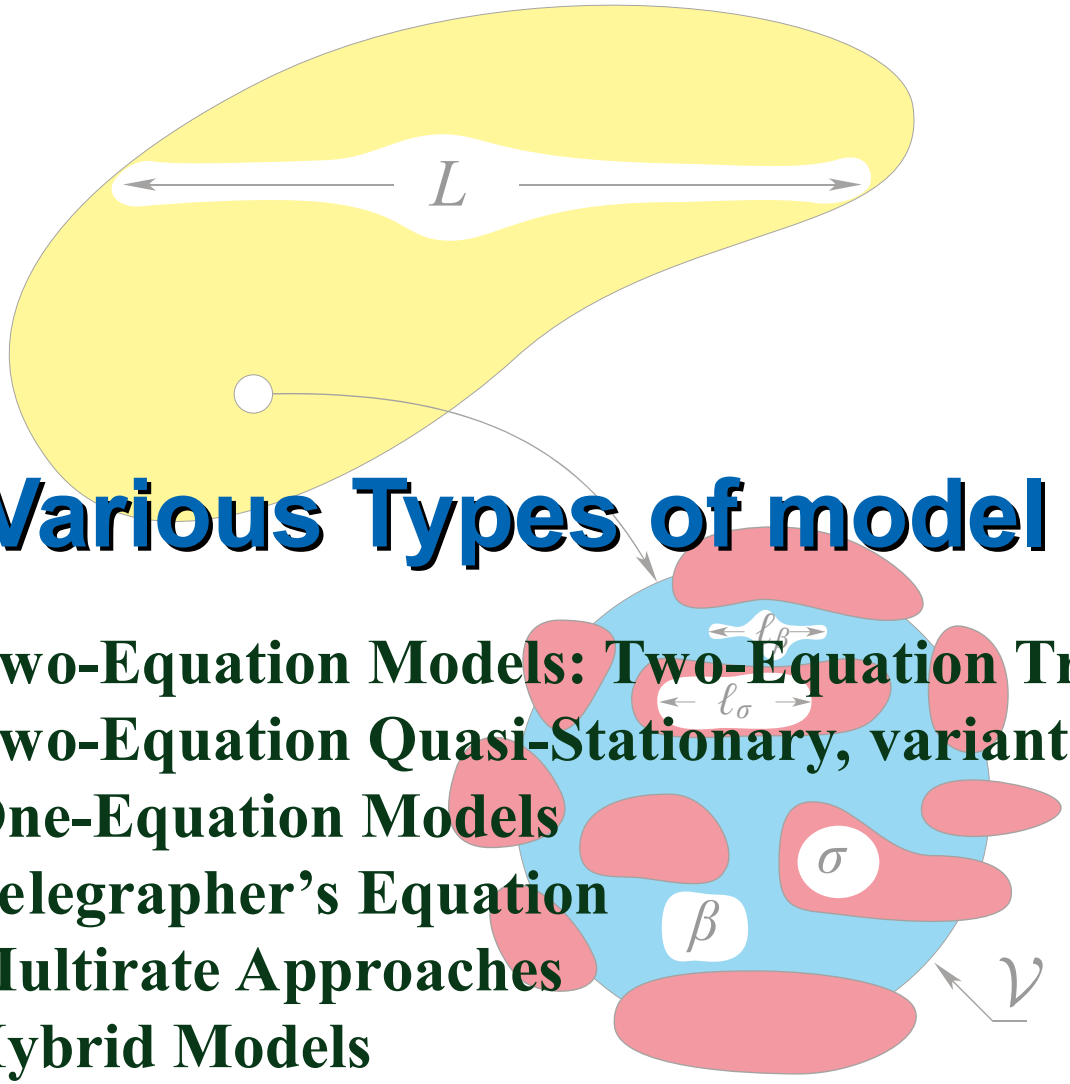


Percolation threshold → OK ; $K_{\text{eff}} \approx (p\text{-}p_c)^{\alpha}$

Sequential upscaling

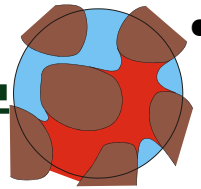
- decreases computer resources requirement, can be easily scripted, ...
- gives additional informations (local heterogeneities, better evaluation of REV, ...)
- no-a priori error estimation with ℓ_u , but end point convergence (not uncommon: see building network approximation)
- requirements:
  - need to use full anisotropy tensors
  - 1st step may require a different upscaling: e.g. Stokes → Darcy → large-scale Darcy
- Alternative: PDE structure adapted for each sub-unit. Not very practical?

see review in *Davit, Y., Quintard, M., 2015. Handbook of Porous Media, in: Vafai, K. (Ed.), Taylor & Francis*.



Various Types of model

- Two-Equation Models: Two-Equation Transient, Two-Equation Quasi-Stationary, variants
- One-Equation Models
- Telegrapher's Equation
- Multirate Approaches
- Hybrid Models
- Etc...



Various types of model, illustrated by the Heat Transfer Problem

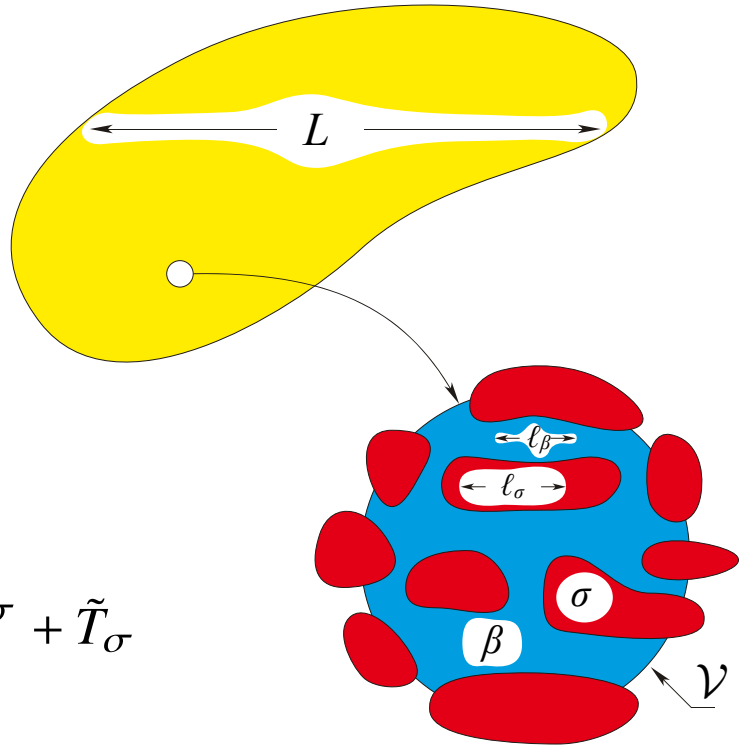
$$\left(\rho c_p\right)_\beta \frac{\partial T_\beta}{\partial t} + \left(\rho c_p\right)_\beta \mathbf{v}_\beta . \nabla T_\beta = \nabla . \left(k_\beta \nabla T_\beta\right) \quad \text{in } V_\beta$$

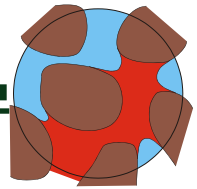
B.C.1 $\quad T_\beta = T_\sigma \quad \text{at } A_{\beta\sigma}$

B.C.2 $\quad -\mathbf{n}_{\beta\sigma} . k_\beta \nabla T_\beta = -\mathbf{n}_{\beta\sigma} . k_\sigma \nabla T_\sigma$

$$(\rho c_p)_\sigma \frac{\partial T_\sigma}{\partial t} = \nabla . (k_\sigma \nabla T_\sigma) \quad \text{in } V_\sigma$$

$$T_\beta = \gamma_\beta \left\langle T_\beta \right\rangle^\beta + \tilde{T}_\beta \qquad T_\sigma = \gamma_\sigma \langle T_\sigma \rangle^\sigma + \tilde{T}_\sigma$$





Macro-scale Temperatures

- **Temperature not additive: ~OK to use phase average**

$$\mathcal{T}_\beta = \left\langle T_\beta \right\rangle^\beta = \frac{1}{\mathcal{V}_\beta} \int_{\mathcal{V}_\beta} T_\beta \, dV$$

$$\mathcal{T}_\sigma = \langle T_\sigma \rangle^\sigma = \frac{1}{\mathcal{V}_\sigma} \int_{\mathcal{V}_\sigma} T_\sigma \, dV$$

- **Mixture Temperature**

$$\langle T \rangle^{\beta\sigma} = \frac{\left(\varepsilon_\beta (\rho c_p)_\beta \left\langle T_\beta \right\rangle^\beta + \left(\rho c_p \right)_\sigma \langle T_\sigma \rangle^\sigma \right)}{\left(\varepsilon_\beta (\rho c_p)_\beta + \varepsilon_\sigma \left(\rho c_p \right)_\sigma \right)}$$

- **Phenomenology**
  - **Contrast of parameters → different regimes**
  - **Local equilibrium :**

$$\left\langle T_\beta \right\rangle^\beta = \langle T_\sigma \rangle^\sigma = \langle T \rangle = \langle T \rangle^{\beta\sigma}$$

  - **Non-equilibrium models**

I - Local Equilibrium → 1-Eq model

$\left\langle T_\beta \right\rangle^\beta = \langle T_\sigma \rangle^\sigma = \langle T \rangle = \langle T \rangle^{\beta\sigma}$ (Carbonell & Whitaker, 84; Nozad et al, 85; …)

$$\varepsilon_\beta \left(\rho c_p\right)_\beta \left\langle T_\beta \right\rangle^\beta + \varepsilon_\sigma \left(\rho c_p\right)_\sigma \langle T_\sigma \rangle^\sigma = \left(\rho c_p\right)^* \langle T \rangle \qquad \left(\rho c_p\right)^* = \varepsilon_\beta \left(\rho c_p\right)_\beta + \varepsilon_\sigma \left(\rho c_p\right)_\sigma$$

Closure: $\tilde{T}_\beta = \mathbf{b}_\beta . \nabla \langle T \rangle + O(\ell^2/L^2)$ $\tilde{T}_\sigma = \mathbf{b}_\sigma . \nabla \langle T \rangle + O(\ell^2/L^2)$

$$\left(\rho c_p\right)^* \frac{\partial \langle T \rangle}{\partial t} + \varepsilon_\beta (\rho c_p)_\beta \mathbf{U}_\beta . \nabla \langle T \rangle = \nabla \cdot \left(\mathbf{K}_{eff} \cdot \nabla \langle T \rangle \right)$$

with:

$$\begin{cases} \mathbf{U}_\beta = \left\langle \mathbf{v}_\beta \right\rangle^\beta \\ \mathbf{K}_{eff} = \left(\varepsilon_\beta k_\beta + \varepsilon_\sigma k_\sigma\right) \mathbf{I} + \underbrace{\frac{(k_\beta - k_\sigma)}{V} \int_{A_{\beta\sigma}} \left(\mathbf{n}_{\beta\sigma} \mathbf{b}_\beta\right) dA}_{\text{tortuosity}} \underbrace{- \left(\rho c_p\right)_\beta \left\langle \tilde{\mathbf{v}}_\beta \mathbf{b}_\beta \right\rangle}_{\text{dispersion}} \end{cases}$$

II - Local Non-Equilibrium: Various closures for 2-Eq models

- **transient closure (→ convolution product, at least in time): retardation and memory effects!**

$$\tilde{T}_\beta = -\frac{\partial s_\beta}{\partial t} * \left(\left\langle T_\beta \right\rangle^\beta - \langle T_\sigma \rangle^\sigma \right) + \frac{\partial \mathbf{b}_{\beta\beta}}{\partial t} * \nabla \left\langle T_\beta \right\rangle^\beta + \frac{\partial \mathbf{b}_{\beta\sigma}}{\partial t} * \nabla \langle T_\sigma \rangle^\sigma + \ldots$$

$$\tilde{T}_\sigma = +\frac{\partial}{\partial t} s_\sigma * \left(\langle T_\sigma \rangle^\sigma - \left\langle T_\beta \right\rangle^\beta \right) + \frac{\partial \mathbf{b}_{\sigma\beta}}{\partial t} * \nabla \left\langle T_\beta \right\rangle^\beta + \frac{\partial \mathbf{b}_{\sigma\sigma}}{\partial t} * \nabla \langle T_\sigma \rangle^\sigma + \ldots$$

- **quasi-steady closure**

$$\tilde{T}_\beta = -s_\beta \left(\left\langle T_\beta \right\rangle^\beta - \langle T_\sigma \rangle^\sigma \right) + \mathbf{b}_{\beta\beta} . \nabla \left\langle T_\beta \right\rangle^\beta + \mathbf{b}_{\beta\sigma} . \nabla \langle T_\sigma \rangle^\sigma + \ldots$$

$$\tilde{T}_\sigma = +s_\sigma \left(\langle T_\sigma \rangle^\sigma - \left\langle T_\beta \right\rangle^\beta \right) + \mathbf{b}_{\sigma\beta} . \nabla \left\langle T_\beta \right\rangle^\beta + \mathbf{b}_{\sigma\sigma} . \nabla \langle T_\sigma \rangle^\sigma + \ldots$$

- **other … Hsu (1999), Nakayama, ...** ***DeGroot & Straatman, 2011***

$$\tilde{T}_\beta = -s_\beta \left(\left\langle T_\beta \right\rangle^\beta - \langle T_\sigma \rangle^\sigma \right) + \mathbf{b}_\beta . \nabla \left\langle T_\beta \right\rangle^\beta + \ldots$$

- **n-th order closure (see Davit and Quintard, 2014, for n=2)**

Local Non-Equilibrium Models: 1st order 2-Eq model

- **Volume averaging theory, 1st order, quasi-steady closure**

  (Carbonell & Whitaker, 84; Zanotti & Carbonell, 84; Quintard & Whitaker, 93, 95, 97; Quintard et al., 96; ……)

$$\varepsilon_\beta \left(\rho c_p\right)_\beta \frac{\partial \left\langle T_\beta \right\rangle^\beta}{\partial t} + \left(\rho c_p\right)_\beta \left\langle \mathbf{v}_\beta \right\rangle . \nabla \left\langle T_\beta \right\rangle^\beta - \ldots = \nabla . \left(\mathbf{K}^*_{\beta\beta} . \nabla \left\langle T_\beta \right\rangle^\beta + \ldots \right) + q_{\beta\sigma}$$

$$\varepsilon_\sigma \left(\rho c_p\right)_\sigma \frac{\partial \left\langle T_\sigma \right\rangle^\sigma}{\partial t} - \ldots = \nabla . \left(\mathbf{K}^*_{\sigma\sigma} . \nabla \left\langle T_\sigma \right\rangle^\sigma + \ldots \right) - q_{\beta\sigma}$$

$$q_{\beta\sigma} = -h_{2eq} \left(\left\langle T_\beta \right\rangle^\beta - \left\langle T_\sigma \right\rangle^\sigma \right) + \ldots$$

heat exchange coefficient

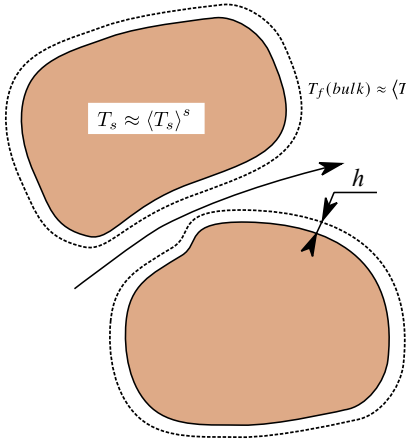
Similar to heuristic models if no non-conventional terms (in red)!

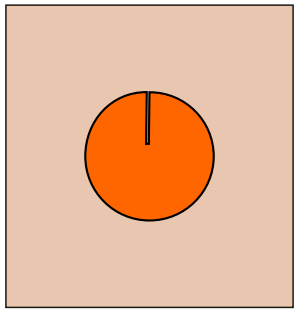
Discussion about exchange coefficient

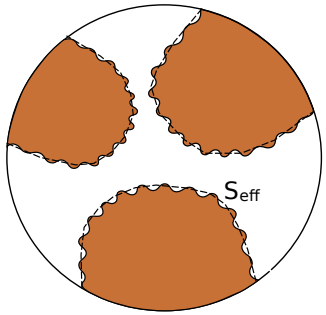
- exchange term has retardation and memory effect
  - $\rightarrow$ no intrinsinc value for $h_{2\mathrm{eq}}$
  - $h_{2\mathrm{eq}}(t)$ is not a correct implementation
- film theory?

$h_{2eq} \neq h\, a_v$ i.e., h and a_v are not independent

a_v may not be a relevant parameter





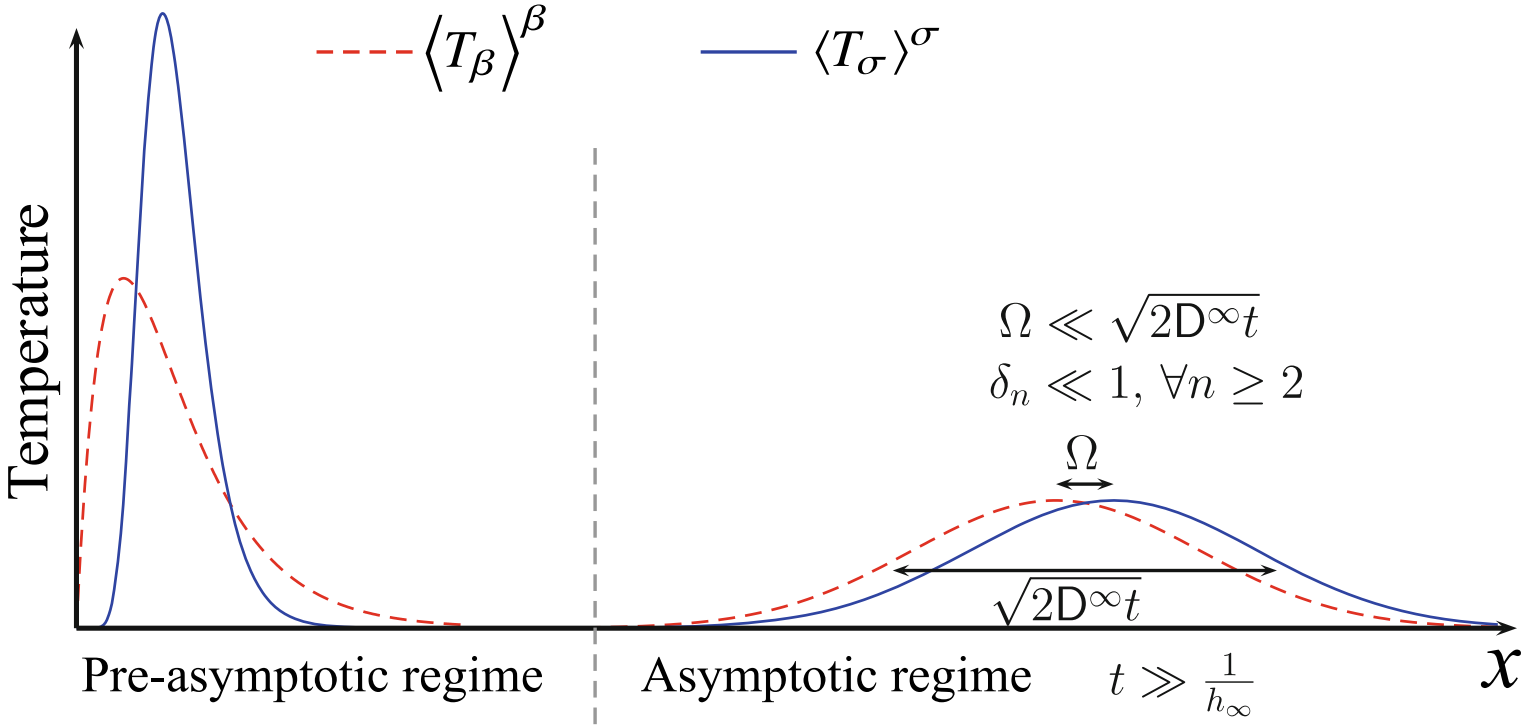


Various estimates for the 1st order exchange coefficient (diffusive case)!

Consequence: various values from inverse methods with ≠ objective functions

	Stratified System	2D-Rectangular System	3D-Parallelepiped System
Asymptotic Value (Linked to 1st eigenvalue)	$\pi^2 k_\sigma / l^2$	$\pi^2 k_\sigma \left(\frac{2}{l^2}\right)$	$\pi^2 k_\sigma \left(\frac{3}{l^2}\right)$
Warren & Root (1963) (Parabolic profile, also literature on LDF models, Liaw et al. (1979))	$12 k_\sigma / l^2$	$16 k_\sigma \left(\frac{2}{l^2}\right)$	$20 k_\sigma \left(\frac{3}{l^2}\right)$
Kazemi et al. (1976, 1992) (Linear Hat profile)	$4 k_\sigma / l^2$	$4 k_\sigma \left(\frac{1}{l_x^2}+\frac{1}{l_y^2}\right)$	$4 k_\sigma \left(\frac{1}{l_x^2}+\frac{1}{l_y^2}+\frac{1}{l_z^2}\right)$
Quintard & Whitaker (1992) (Linked to harmonic mean of eigenvalues!)	$12 k_\sigma / l^2$	$14.22 k_\sigma \left(\frac{1}{l_x^2}+\frac{1}{l_y^2}\right)$	$16.54 k_\sigma \left(\frac{1}{l_x^2}+\frac{1}{l_y^2}+\frac{1}{l_z^2}\right)$

III - 2-Eq Asymptotic Behavior (mixture temperature)



from Zanotti & Carbonell, 1984; Davit et al., 2010 (moment analysis)

2-Eq Asymptotic Behavior (mixture temperature)

$$\left(\varepsilon_\beta \left(\rho c_p\right)_\beta \left\langle T_\beta \right\rangle^\beta + \varepsilon_\sigma \left(\rho c_p\right)_\sigma \left\langle T_\sigma \right\rangle^\sigma\right) = \left(\varepsilon_\beta \left(\rho c_p\right)_\beta + \varepsilon_\sigma \left(\rho c_p\right)_\sigma\right) \left\langle T \right\rangle^{\beta\sigma}$$

- *$t \to \infty$ for a semi- or infinite medium (see Zanotti & Carbonell, 1984; Davit et al., 2010)*:

$$\left(\varepsilon_\beta \left(\rho c_p\right)_\beta + \varepsilon_\sigma \left(\rho c_p\right)_\sigma\right) \frac{\partial \left\langle T \right\rangle^{\beta\sigma}}{\partial t} + \varepsilon_\beta \left(\rho c_p\right)_\beta U_\beta \frac{\partial \left\langle T \right\rangle^{\beta\sigma}}{\partial x} = \left(K_\infty^*\right)_{xx} \frac{\partial^2 \left\langle T \right\rangle^{\beta\sigma}}{\partial x^2}$$

$$\left(K_\infty^*\right)_{xx} = \left(K_{\beta\beta}^*\right)_{xx} + \left(K_{\beta\sigma}^*\right)_{xx} + \left(K_{\sigma\beta}^*\right)_{xx} + \left(K_{\sigma\sigma}^*\right)_{xx} + \frac{\left(\varepsilon_\beta \left(\rho c_p\right)_\beta \varepsilon_\sigma \left(\rho c_p\right)_\sigma U_\beta\right)^2}{h_{2eq} \left(\varepsilon_\beta \left(\rho c_p\right)_\beta + \varepsilon_\sigma \left(\rho c_p\right)_\sigma\right)^2}$$

$$\neq K_{eff} = K_{\beta\beta}^* + K_{\beta\sigma}^* + K_{\sigma\beta}^* + K_{\sigma\sigma}^*$$

- → good test for the choice of … h_{2eq}!

IV - 1-Eq Non-Equilibrium Model

(Chella et al., 1998; Moyne et al., 2000; Quintard et al., 2001; Davit et al., 2010; ~Brenner's method)

- **Mixture Temperature:**

$$\langle T \rangle^{\beta\sigma} = \frac{\left(\varepsilon_\beta (\rho c_p)_\beta \left\langle T_\beta \right\rangle^\beta + \left(\rho c_p \right)_\sigma \langle T_\sigma \rangle^\sigma \right)}{\left(\varepsilon_\beta (\rho c_p)_\beta + \varepsilon_\sigma \left(\rho c_p \right)_\sigma \right)}$$

- **New decomposition:** $\hat{T}_\beta = T_\beta - \langle T \rangle^{\beta\sigma}$
- **Specific Closure:**

$$\hat{T}_\beta = \mathbf{b}_\beta^\infty . \nabla \langle T \rangle^{\beta\sigma} \qquad \hat{T}_\sigma = \mathbf{b}_\sigma^\infty . \nabla \langle T \rangle^{\beta\sigma}$$

- **same equation and effective property as asymptotic eq.**

  $\rightarrow$ Direct Estimation of $\mathbf{K}_\infty^*$ (see proof in Davit et al., 2010, if proper closure problem!)

- **see Moyne et al. for relation with homogenization theory**

V - Better Non-Equilibrium models (N-eq., multi-rate models)

- **Multi-rate (Brusseau et al., 1989;…); N-equation (Landereau et al., 1998) → a practical alternative to time convolution**

$$\varepsilon_\beta (\rho c_p)_\beta \frac{\partial \langle T_\beta \rangle^\beta}{\partial t} = \nabla \cdot \left(K_\beta \nabla \langle T_\beta \rangle^\beta \right) - \sum_n b_n \left(\langle T_\beta \rangle^\beta - T_{\sigma n} \right)$$

$$\varepsilon_\sigma (\rho c_p)_\sigma \frac{\partial T_{\sigma n}}{\partial t} = -k_\sigma \lambda_n \left(T_{\sigma n} - \langle T_\beta \rangle^\beta \right) \qquad n = 1, 2, ..$$

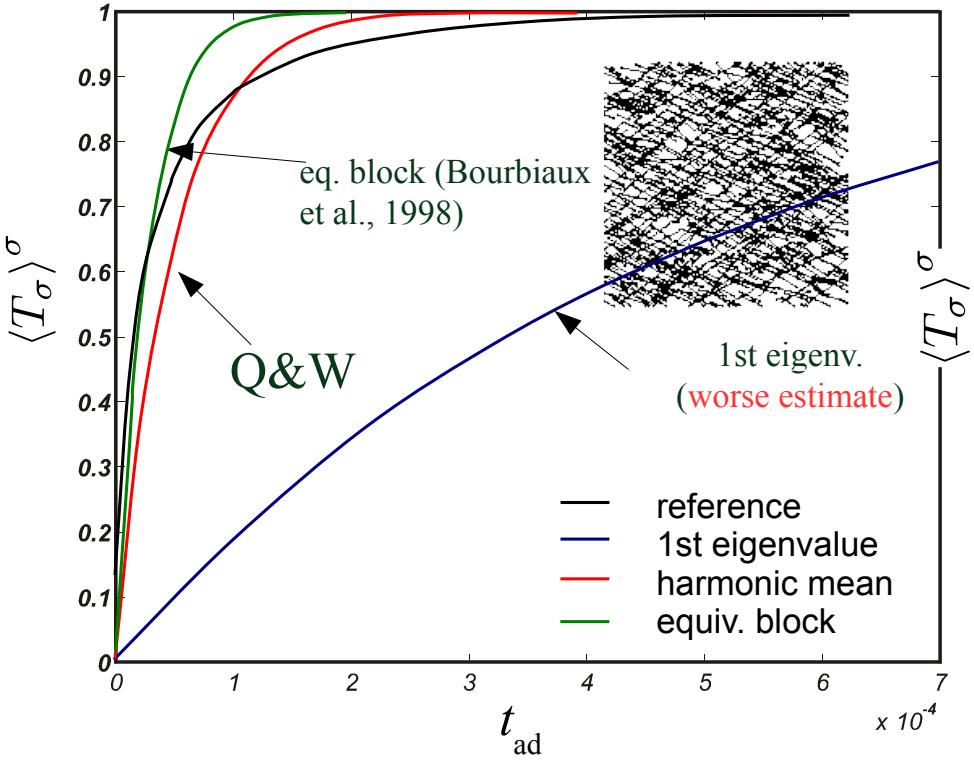
Example: 3-eqs

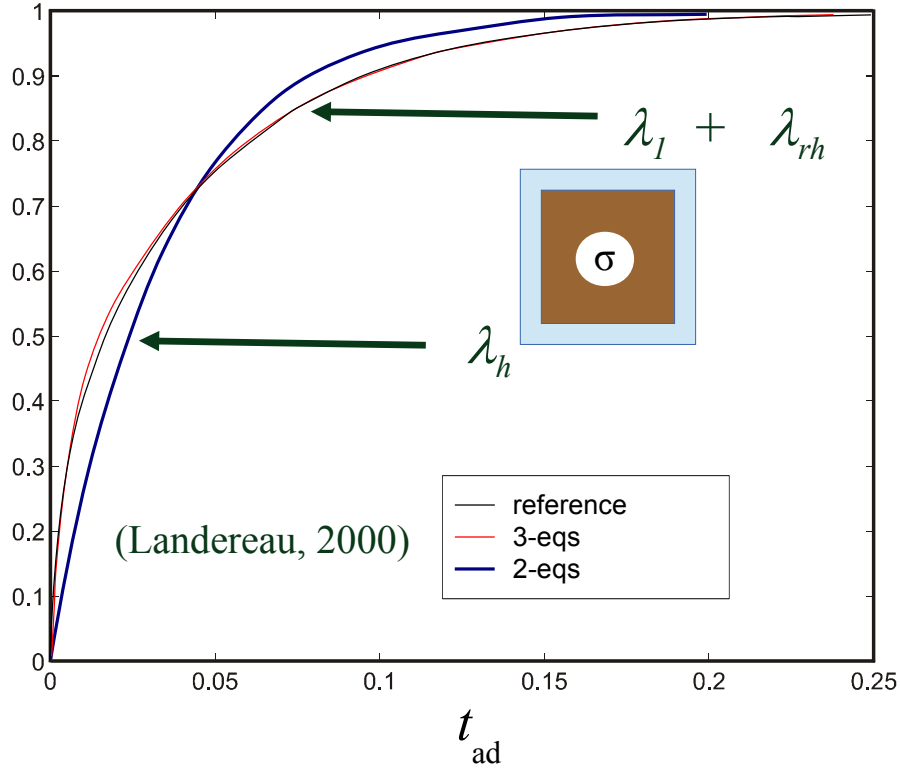
$T_{\sigma 1}$, $T_{\sigma r}$

with λ_1 , λ_r (from the harmo. mean of the remaining eigenv.)

Examples: fractured media

(also for Darcy's law with slightly compressible fluid)





Tests with various h_{2eq}

Test with 3-Eq model

VI - Mixed (or Hybrid) Model

(diffusion, $k_\sigma \ll k_\beta$, dispersed σ-phase; De Swaan, 1976; …..)

$$\langle T_\beta \rangle^\beta \underbrace{+\tilde{T}_\beta}_{O(\frac{l_\beta}{L}\langle T_\beta \rangle^\beta)} = T_\sigma \Rightarrow \underbrace{\langle T_\beta \rangle^\beta}_{\text{macro-scale}} = \underbrace{T_\sigma}_{\text{micro-scale}}$$

Macro-

$$\varepsilon_\beta (\rho C_p)_\sigma \frac{\partial \langle T_\beta \rangle^\beta}{\partial t} = \nabla . \left(\mathbf{K}^*_\beta . \nabla \langle T_\beta \rangle^\beta \right) - \varphi_{\beta\sigma}$$

Micro-

$$(\rho c_p)_\sigma \frac{\partial T_\sigma}{\partial t} = \nabla . (k_\sigma \nabla T_\sigma) \quad \text{in } V_\sigma \qquad T_\sigma = \langle T_\beta \rangle^\beta \text{ , at } A_{\beta\sigma}$$

general solution:

$$T_\sigma(\mathbf{x}, t) = \int_0^t \left. \frac{\partial \langle T_\beta \rangle^\beta}{\partial t} \right|_{t-\tau} \overline{T}_\sigma(\mathbf{x}, \tau)\, d\tau$$

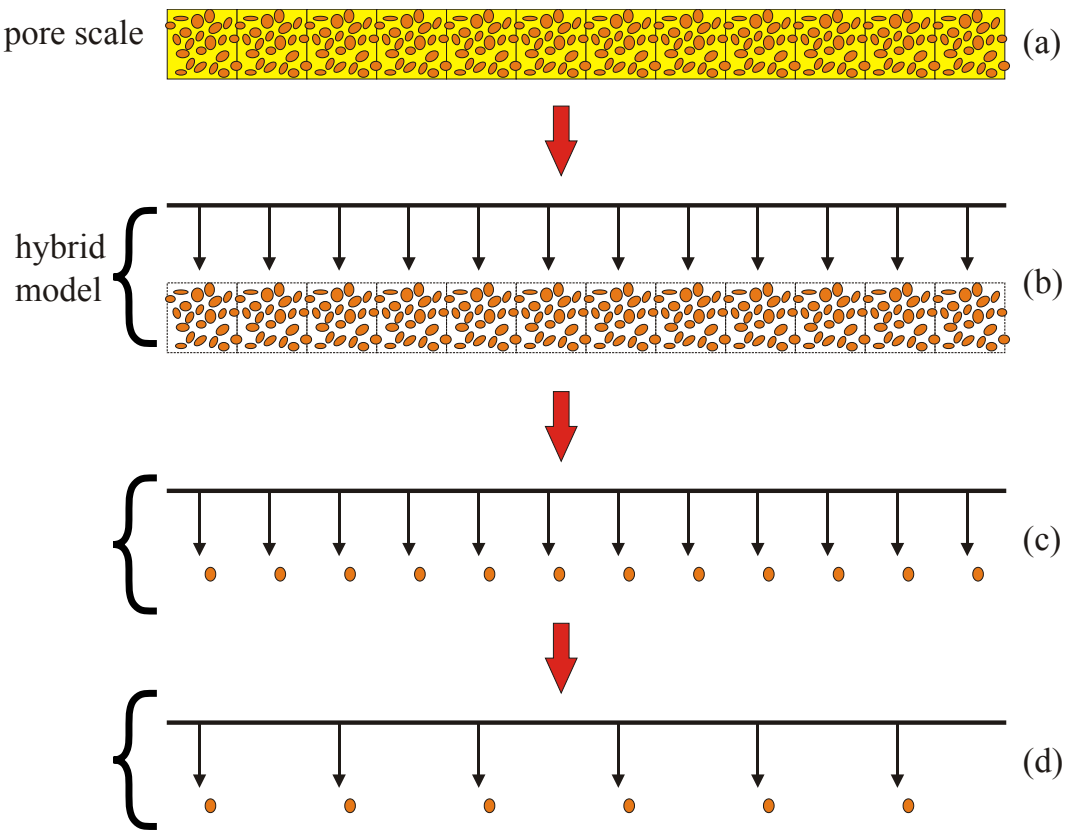
→ involves spectrum of eigenvalues & eigenfunctions → *h*(*t*, *BC*, *IC*)!

Mixed (or Hybrid) Model: Practical Implementation

-Direct Numerical Simulation (Heavy computations)

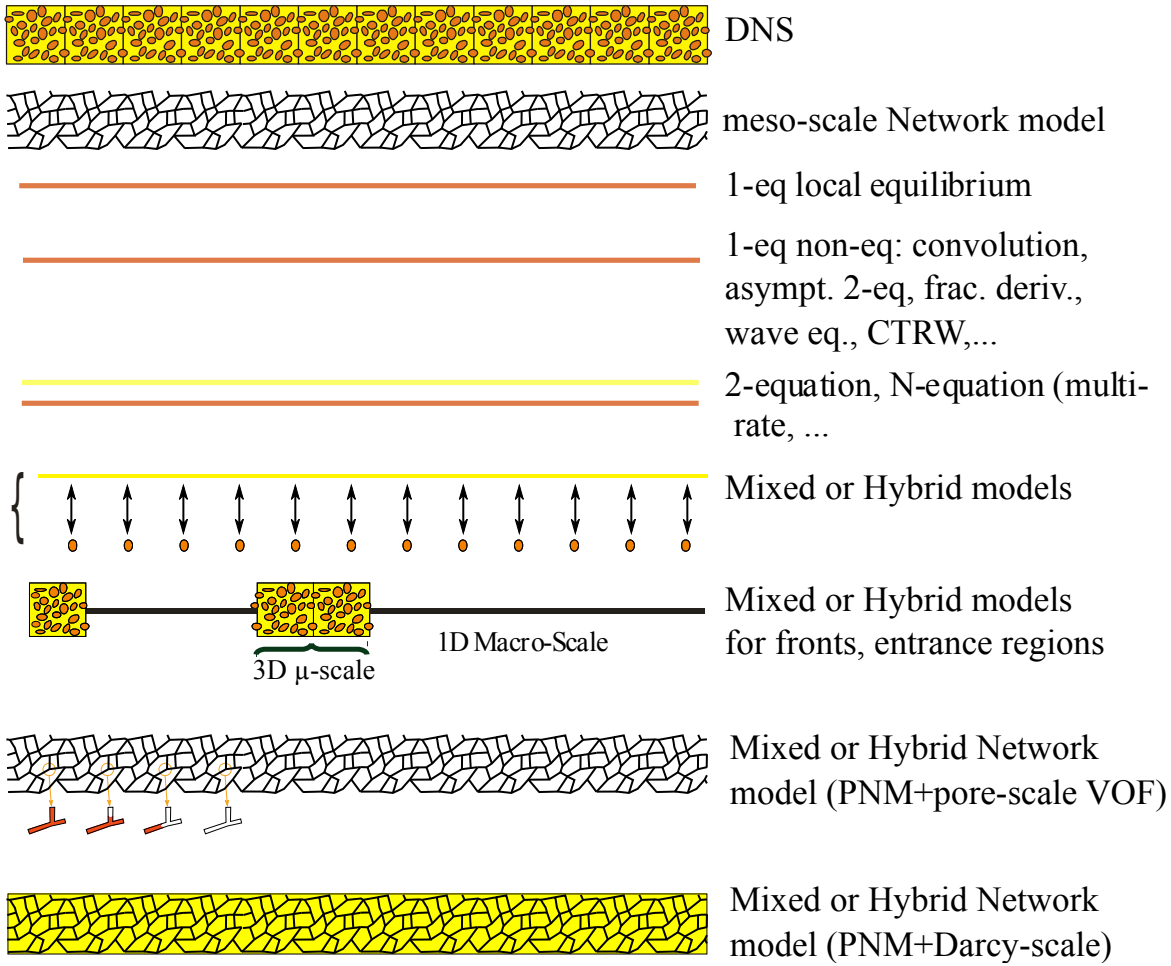
-Mixed Model, Full UC (still Heavy Comp.)

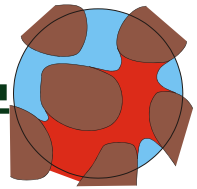
-Mixed Model, Representative Matrix Block,…



…in some cases Analytical Solutions may be available

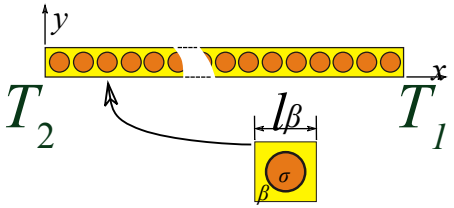
Synoptic of various models

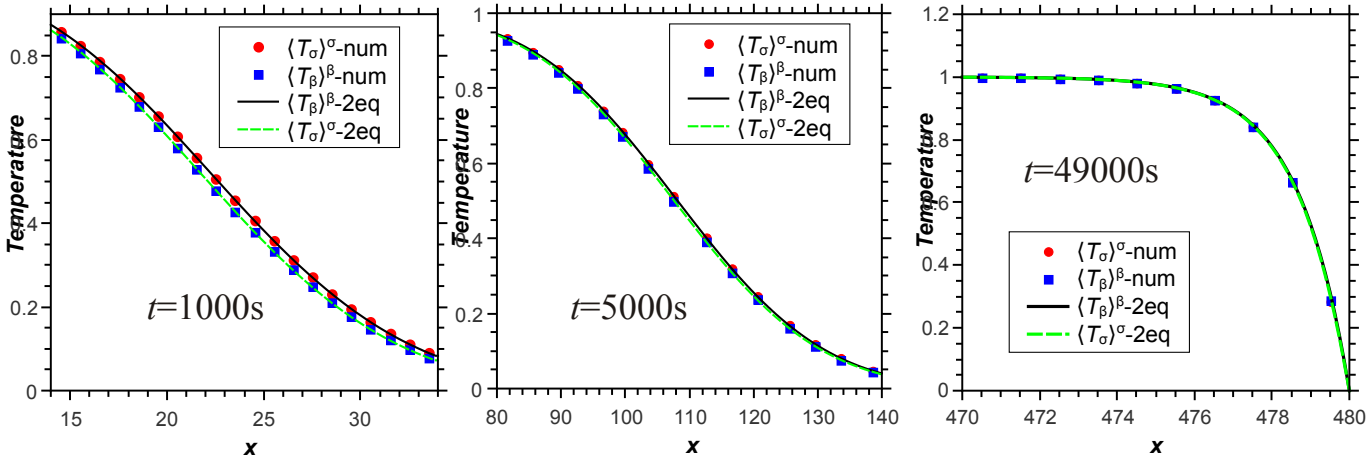




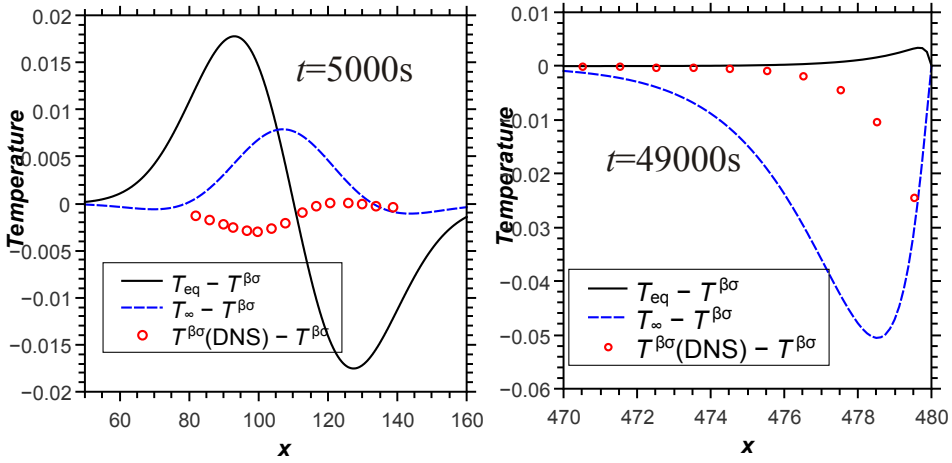
Important: transitions between the various models!

(Davarzani et al., 2010; Davit & Quintard, 2014)





- t~0 non-homogenizable or specific treatment
- t>0 LNE models
- t>>0 (if enough length): 1-Eq asymptotic model
- t → ∞ (revert to 1eq-LE if finite domain, because of Dirichlet condition)



Conclusions: How to handle multi-scale systems?

- Popular picture: REV, upscaling, macro-scale equations and effective properties
- Sequential upscaling: may be use to built approximations for systems without the need of a REV
- Complexity often results in different types of models (fully closed models, mixed models, N-equations, hybrid models, etc...)
- not discussed today: highly non-linear or coupled problems, effective boundary conditions, etc...