

4th Cargèse Summer School, 2018

Non-Newtonian Flows in Porous Media: upscaling problems

https://www.dropbox.com/s/mcgg0ifpogsznv2/non_newtonian_V00.pdf?dl=0

**Davit Y.¹, Zami-Pierre F.^{1,2}, de Loubens
R.² and Quintard M.¹**

¹Institut de Mécanique des Fluides de Toulouse (IMFT) -
Université de Toulouse, CNRS-INPT-UPS, Toulouse FRANCE

²**Total**, CSTJF, Avenue Larribau, 64018 Pau, France

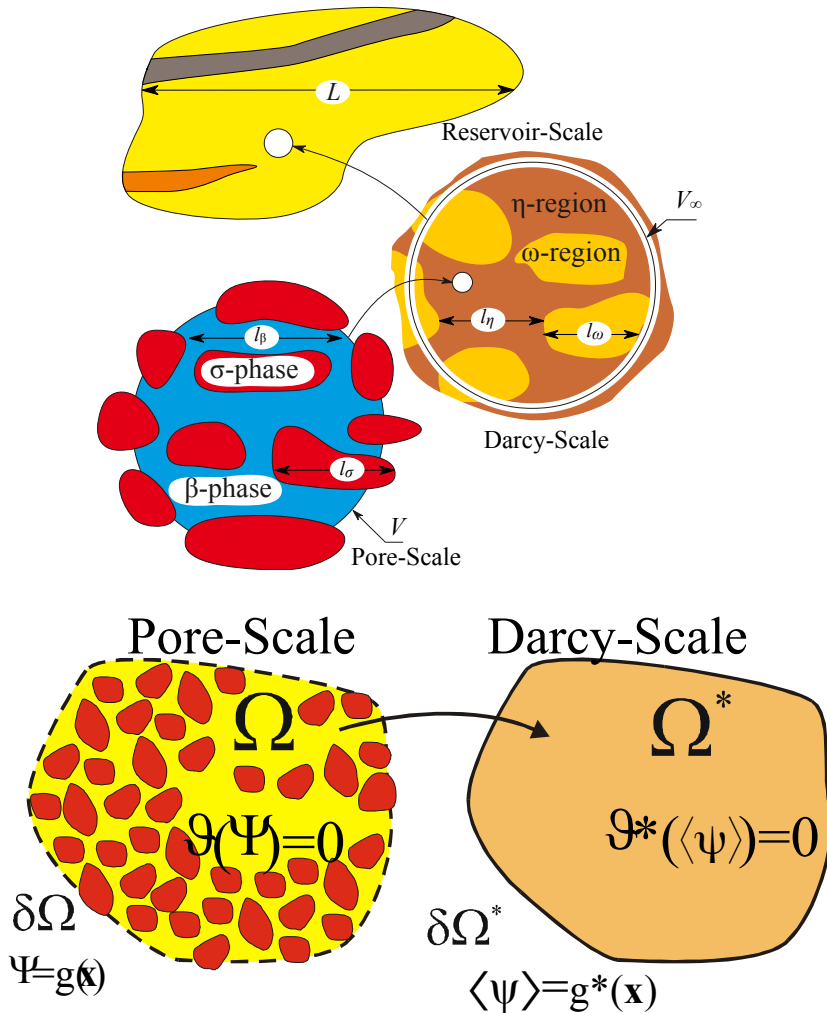


Objective/Outline

- *Motivation: flow of polymer solutions, question about heuristic models in Res. Engng*
- **Upscaling**
 - Introduction (generalized Stokes)
 - Transition
 - Induced anisotropy, effect of disorder, effect of size of the UC, ...
- **Further problems: exclusion zone, viscoelastic**
- **Conclusions**



Multi-Scale Analysis



- Sequential multi-scale pattern
- Used in DRP, Res. Engng, Hydro., etc...
- Objectives of macro-scale theories:
 - Smoothing operator $\langle . \rangle \rightarrow$ Macro variables, Eqs & BCs
 - Micro-macro link \rightarrow Determination of Effective Properties
- Needs Scale Separation:
 - $l_\beta, l_\sigma \ll \text{REV?} \ll L$
 - (process dependent)

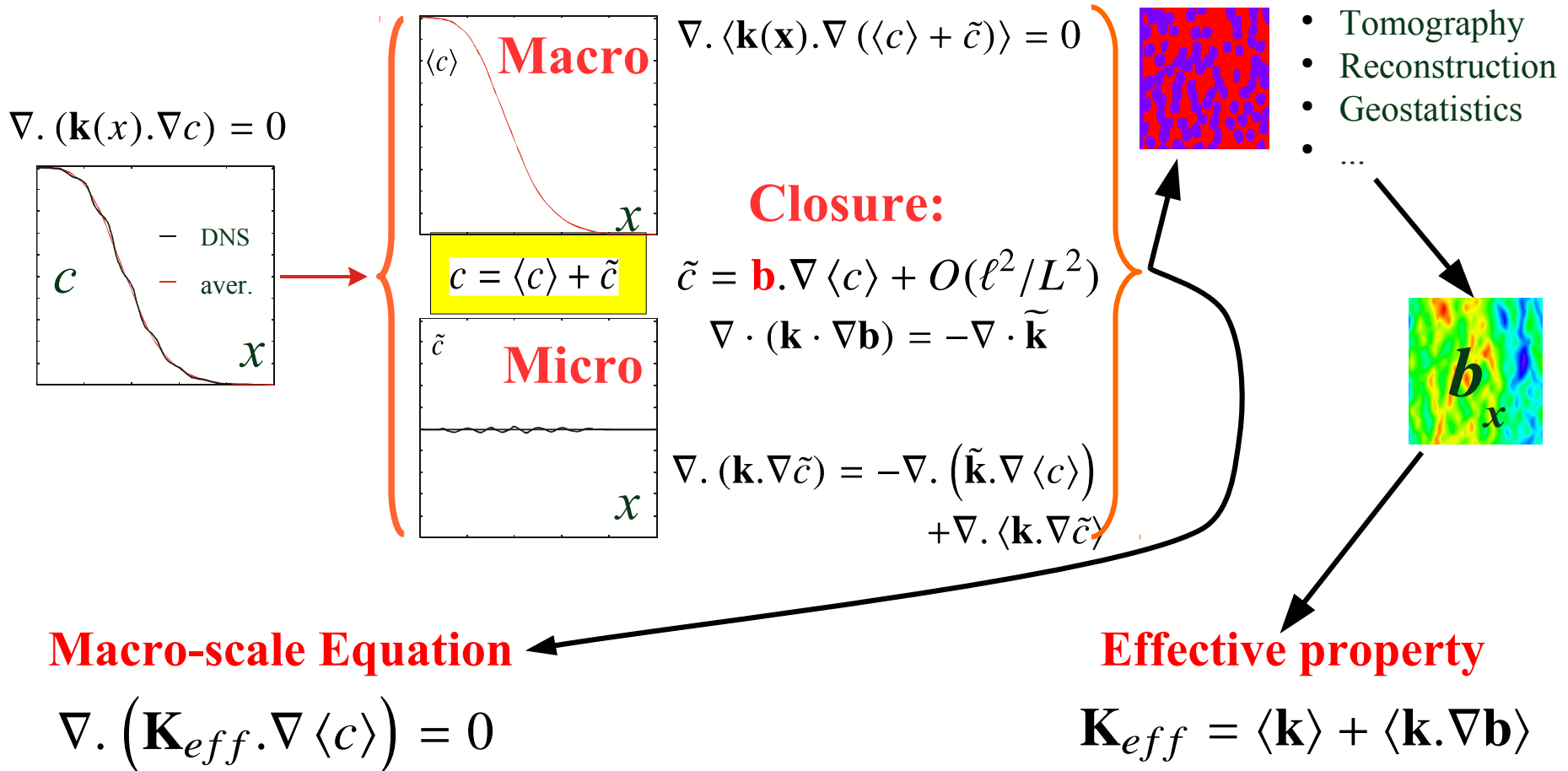


Multi-Scale Analysis: Upscaling Techniques

- **Form of the equations?**
 - averaging and TIP (Marle, Gray, Hassanizadeh, ...)
 - averaging and closure (Whitaker, ...)
 - homogenization (Bensoussan et al., Sanchez-Palencia, Tartar, ...), also “closure”
 - stochastic approaches (Dagan, Gelhar, ...)
- **Effective properties calculations?**
 - Assuming the form of Eqs: interpret experiments or DNS
 - Upscaling with “closure” (averaging, homogenization, stochastic): provides *local* Unit Cell problems
- **Many Open Problems: High non-linearities, Strong couplings, Evolving pore-scale structure, ...**



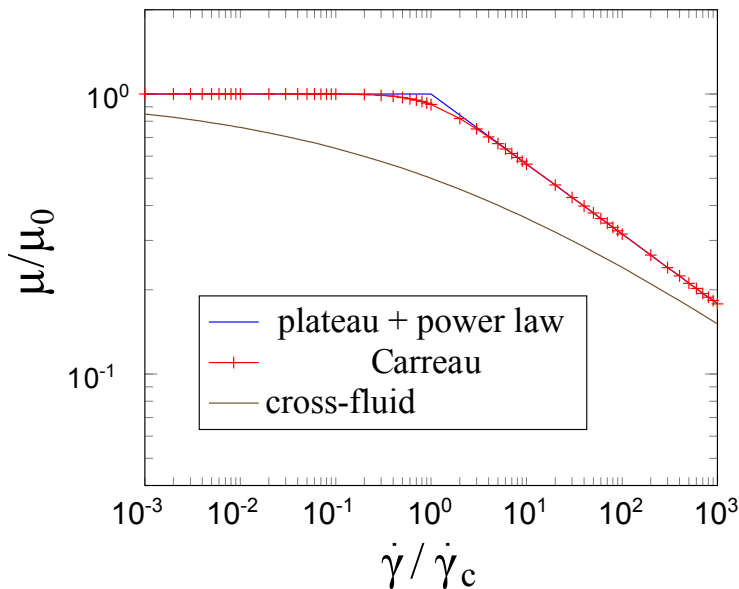
A simple introduction to upscaling with “closure”



Flow of a non-Newtonian fluid

Case of Generalized Stokes equation

- **Pore-Scale problem (Re~0)**



$$\nabla \cdot \left[\mu_\beta (\dot{\gamma}) \left(\nabla \mathbf{v}_\beta + {}^T (\nabla \mathbf{v}_\beta) \right) \right] - \nabla p_\beta + \rho_\beta \mathbf{g} = 0 \quad \text{in } V_\beta$$

$$\nabla \cdot \mathbf{v}_\beta = 0 \quad \text{in } V_\beta ; \quad \mathbf{n}_{\beta\sigma} \cdot \mathbf{v}_\beta = 0 \quad \text{at } A_{\beta\sigma}$$

Rheology:

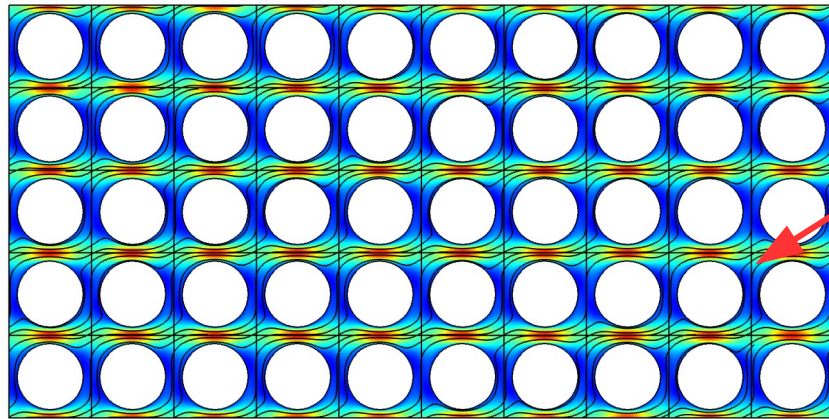
$$\mu_\beta = \mu_0 \hat{\mu}(\dot{\gamma}) \quad \dot{\gamma} = \left\| \frac{1}{2} \left(\nabla \mathbf{v}_\beta + {}^T (\nabla \mathbf{v}_\beta) \right) : \left(\nabla \mathbf{v}_\beta + {}^T (\nabla \mathbf{v}_\beta) \right) \right\|$$

- **Upscaling: (vol. aver. $\langle \psi_\beta \rangle = \varepsilon_\beta \langle \psi_\beta \rangle^\beta$ with $\varepsilon_\beta = V_\beta / V$)?**

$$p_\beta = \langle p_\beta \rangle^\beta + \tilde{p}_\beta ; \quad \mathbf{v}_\beta = \langle \mathbf{v}_\beta \rangle^\beta + \tilde{\mathbf{v}}_\beta$$



Typical local (over a REV) features



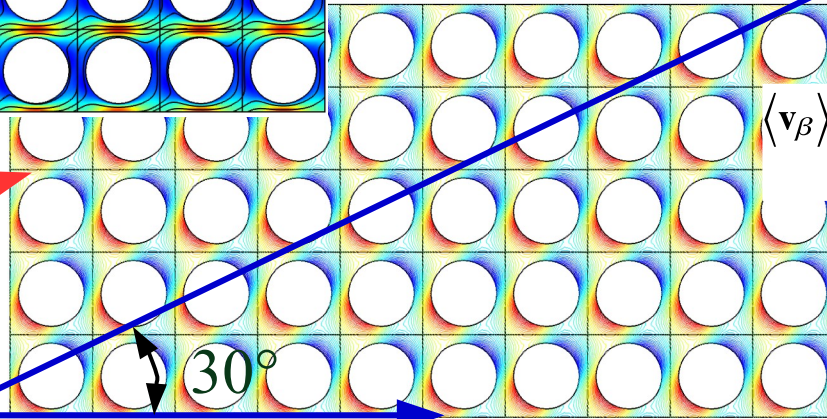
velocity

Remark (far from BCs)

$$\nabla \langle \mathbf{v}_\beta \rangle \approx 0$$

$$\nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g} \approx \text{Constant}$$

Pressure dev.

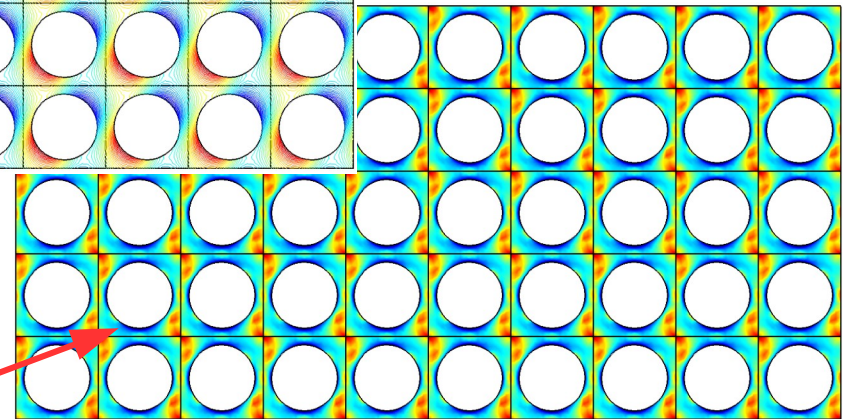


$$\langle \mathbf{v}_\beta \rangle = \underbrace{-\mathbf{K}_{gen}}_{\text{permeance}} (\langle \mathbf{v}_\beta \rangle) \cdot (\nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g})$$

$$\nabla p_\beta - \rho_\beta \mathbf{g} = \nabla \tilde{p}_\beta + \underbrace{\nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g}}_{\text{constant } \mathbf{h}}$$

constant \mathbf{h}

viscosity



Upscaling flow of a non-Newtonian fluid

- Averaging (vol. aver. $\langle \psi_\beta \rangle = \varepsilon_\beta \langle \psi_\beta \rangle^\beta$ with $\varepsilon_\beta = V_\beta / V$)

$$\text{macro} \left\{ \begin{array}{l} \nabla \cdot \langle \mathbf{v}_\beta \rangle = 0 \\ -\varepsilon_\beta \left(\nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g} \right) + \underbrace{\frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \left[\mu_\beta(\tilde{\gamma}) \left(\nabla \tilde{\mathbf{v}}_\beta + {}^\top (\nabla \tilde{\mathbf{v}}_\beta) \right) - \tilde{p}_\beta \right]}_{\text{Closure?}} dA = 0 \end{array} \right. + \dots$$

$$\text{micro} \left\{ \begin{array}{l} 0 = -\nabla \tilde{p}_\beta + \nabla \cdot \left(\mu_\beta \left(\nabla \tilde{\mathbf{v}}_\beta + \nabla \tilde{\mathbf{v}}_\beta^\top \right) \right) - \left(\nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g} \right) \\ \nabla \cdot (\tilde{\mathbf{v}}_\beta) = 0 \\ \tilde{\mathbf{v}} = -\langle \mathbf{v}_\beta \rangle^\beta \text{ at } A_{\beta\sigma} \end{array} \right.$$

⇒ Problem must be solved for each value of $\langle \mathbf{v}_\beta \rangle^\beta$!



“Closure”?

Under several constraints: scale separation, far from BCs, ...

⇒

Tentatively:

$$\begin{aligned}\tilde{\mathbf{v}}_\beta &= \mathbf{B} \cdot \langle \mathbf{v}_\beta \rangle^\beta + \dots \\ \tilde{p}_\beta &= \mu_0 \mathbf{b} \cdot \langle \mathbf{v}_\beta \rangle^\beta + \dots\end{aligned}$$

$$(\nabla \cdot [\hat{\mu}(\hat{\gamma}) (\nabla \mathbf{B} + {}^\top (\nabla \mathbf{B}))] - \nabla \mathbf{b}) \cdot \langle \mathbf{v}_\beta \rangle^\beta = \langle \nabla \cdot [\hat{\mu}(\hat{\gamma}) (\nabla \mathbf{B} + {}^\top (\nabla \mathbf{B}))] - \nabla \mathbf{b} \rangle^\beta \cdot \langle \mathbf{v}_\beta \rangle^\beta$$

$$(\nabla \cdot \mathbf{B}) \cdot \langle \mathbf{v}_\beta \rangle^\beta = 0 ; \mathbf{B} \cdot \langle \mathbf{v}_\beta \rangle^\beta = -\mathbf{I} \cdot \langle \mathbf{v}_\beta \rangle^\beta \text{ at } A_{\beta\sigma}$$

$$\mathbf{B}(\mathbf{r}) = \mathbf{B}(\mathbf{r} + h\mathbf{e}_i) \text{ and } \mathbf{b}(\mathbf{r}) = \mathbf{b}(\mathbf{r} + h\mathbf{e}_i) \text{ for } i = 1, 2, 3 \text{ (periodicity)}$$

$$\langle \mathbf{b} \rangle = 0$$

$$\text{with } \hat{\gamma} = \left\| (\nabla \mathbf{B} + {}^\top \nabla \mathbf{B}) \cdot \mathbf{e}_\beta \right\| \left\| \langle \mathbf{v}_\beta \rangle^\beta \right\|$$

$$\mathbf{e}_\beta = \langle \mathbf{v}_\beta \rangle^\beta / \left\| \langle \mathbf{v}_\beta \rangle^\beta \right\|$$

⇒ Problem must be solved for each value of $\langle \mathbf{v}_\beta \rangle^\beta$!



A classical story: the linear case and Darcy's law (see Sanchez-Palencia, Whitaker, ...)

- Closure (any solution is a linear combination of elementary solutions for $\langle \mathbf{v}_\beta \rangle^{\beta=e_i}$ for $i=1,2,3$)

$$\begin{aligned}\tilde{\mathbf{v}}_\beta &= \mathbf{B} \cdot \langle \mathbf{v}_\beta \rangle^\beta + \dots \\ \tilde{p}_\beta &= \mu_0 \mathbf{b} \cdot \langle \mathbf{v}_\beta \rangle^\beta + \dots\end{aligned}$$

$$(\nabla \cdot (\nabla \mathbf{B} + {}^\top (\nabla \mathbf{B})) - \nabla \mathbf{b}) = \langle \nabla \cdot (\nabla \mathbf{B} + {}^\top (\nabla \mathbf{B})) - \nabla \mathbf{b} \rangle^\beta$$

$$(\nabla \cdot \mathbf{B}) = 0 ; \mathbf{B} = -\mathbf{I} \text{ at } A_{\beta\sigma} \quad \text{over a UC!}$$

$$\mathbf{B}(\mathbf{r}) = \mathbf{B}(\mathbf{r} + h\mathbf{e}_i) \text{ and } \mathbf{b}(\mathbf{r}) = \mathbf{b}(\mathbf{r} + h\mathbf{e}_i) \text{ for } i = 1, 2, 3 \text{ (periodicity)}$$

$$\langle \mathbf{b} \rangle = 0$$

- Macro-Scale equation and effective properties

Darcy's law:

$$\langle \mathbf{v}_\beta \rangle = -\frac{1}{\mu_0} \mathbf{K}_0 \cdot (\nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g})$$

$$\text{Intrinsic permeability: } \mathbf{K}_0^{-1} = \frac{1}{V} \int_{V_\beta} (\nabla \cdot (\nabla \mathbf{B} + {}^\top (\nabla \mathbf{B})) - \nabla \mathbf{b}) dV$$

Important: Proof of symmetry of \mathbf{K}_0 requires periodicity!



Calculations of the permeability

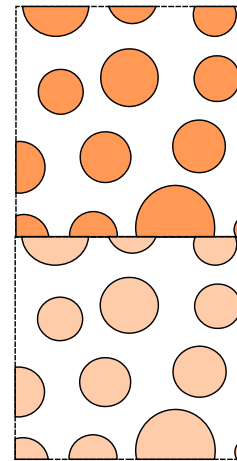
Case of “diffusion” problem: e.g., permeability, effective diffusion

- 3 possibilities

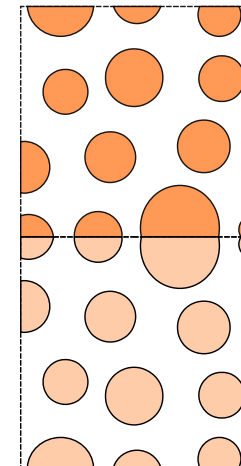
- Initial closure problem
- Transformation of closure problem into ~Stokes with source term and periodic pressure and velocity
- “permeameters”: non-periodicity

- Making image periodic?

- I: Percolation problem
- II: Loss of anisotropy
- III: potentially various bias



I



II

- thin layers + periodicity
- Eff. Medium
-

III

See discussion in Guibert et al., 2015

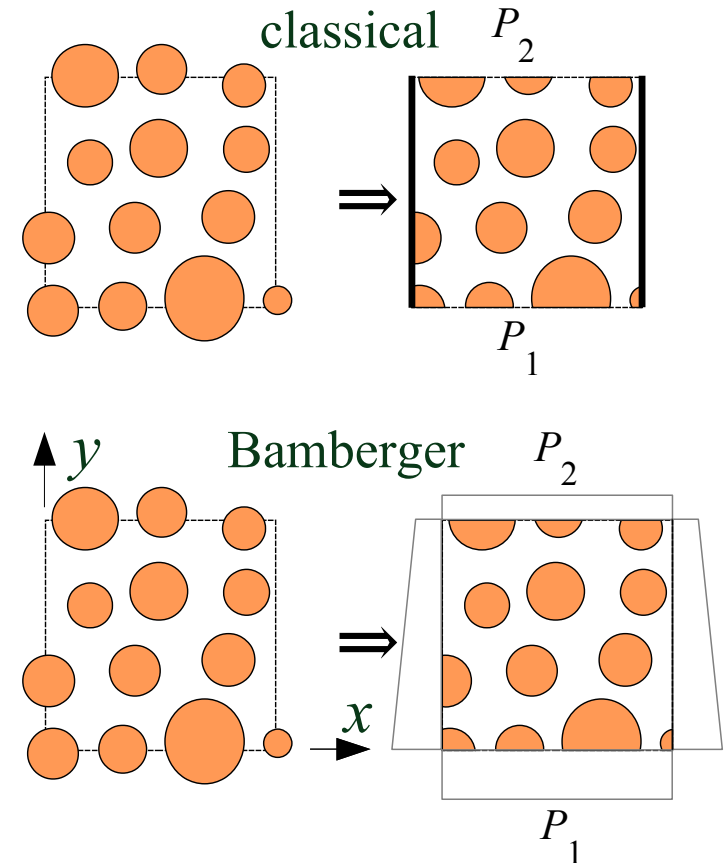


Calculations over non-periodic images

- “permeameters”
 - All methods have bias
 - $\langle v_x \rangle^\beta \neq 0$
 - $K_{xy} \neq K_{yx}$

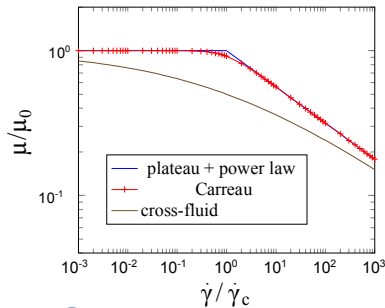
Note: minimal bias if large sample and anisotropy along the axis

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



Non-Linear Case: Non-Newtonian Fluid

- Fluid rheology



PLCO

$$\mu = \begin{cases} \mu_0 & \text{if } \dot{\gamma} < \dot{\gamma}_c, \\ \mu_0 \left(\frac{\dot{\gamma}}{\dot{\gamma}_c}\right)^{n-1} & \text{else.} \end{cases}$$

- No generic closure independent of fluid velocity! Generic macro-scale law:

$$\langle \mathbf{v}_\beta \rangle = - \underbrace{\mathbf{K}_{gen}(\langle \mathbf{v}_\beta \rangle)}_{\text{permeance}} \cdot \left(\nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g} \right)$$

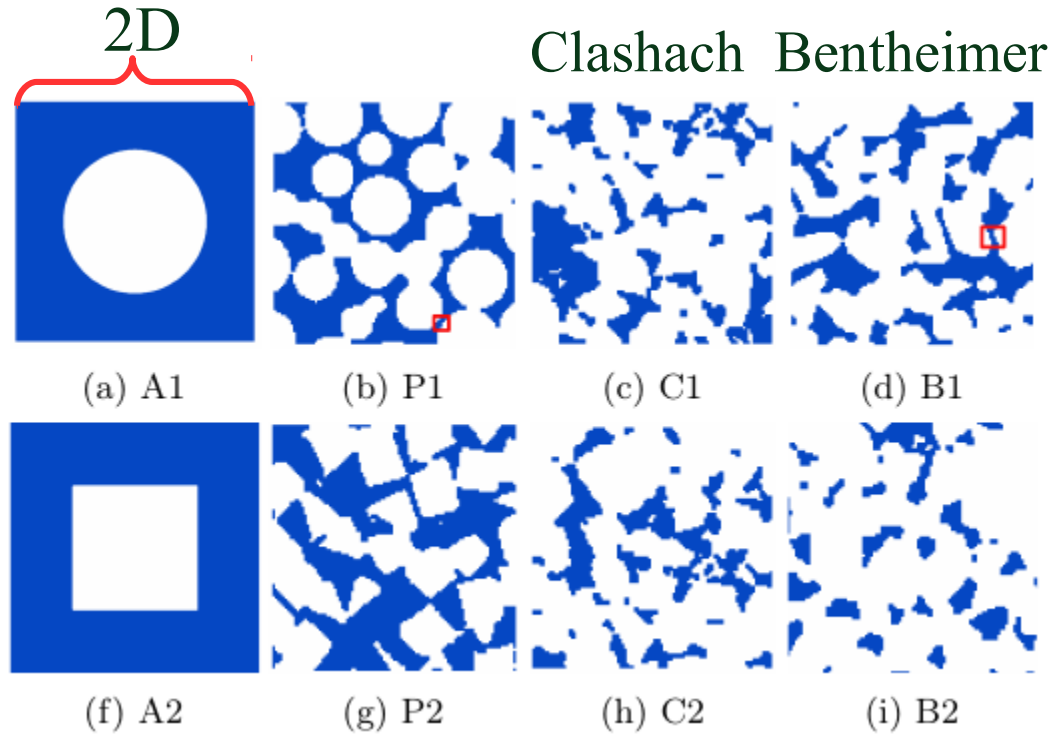
- Representation as a deviation from Darcy's law

$$\langle \mathbf{v}_\beta \rangle = - \frac{1}{\mu_0} k_n \mathbf{P} \cdot \underbrace{\mathbf{K}_0 \cdot \left(\nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g} \right)}_{\text{newtonian velocity}}$$

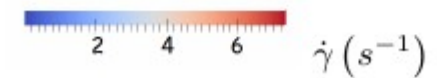
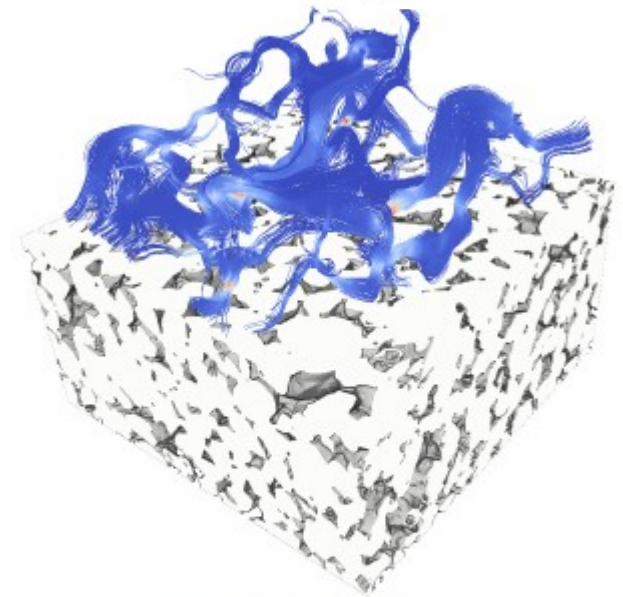
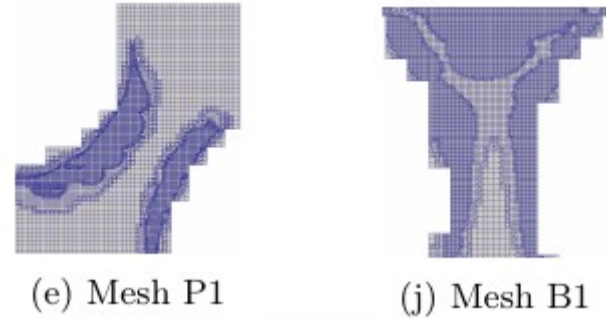
– k_n , \mathbf{P} (rotation “matrix”): depend on $\langle \mathbf{v}_\beta \rangle^\beta$ (modulus and orientation)



Test cases



Needs very fine grid!



(k) B1

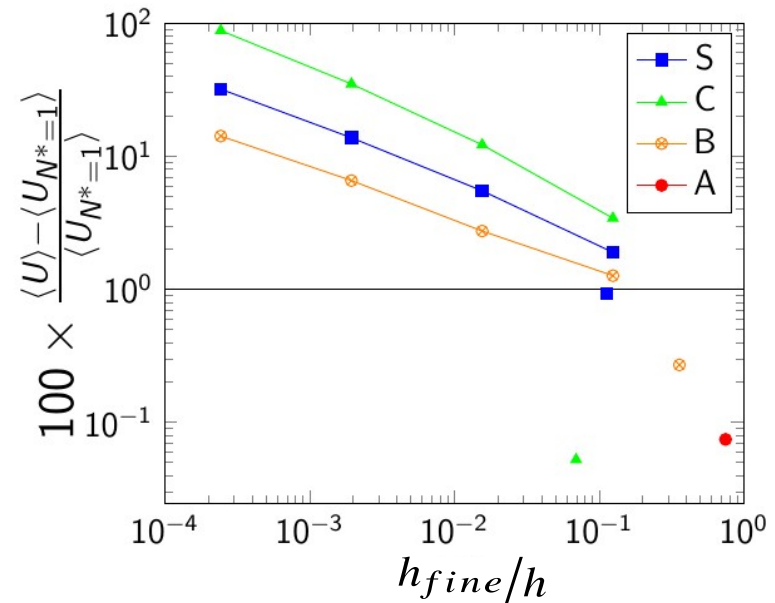
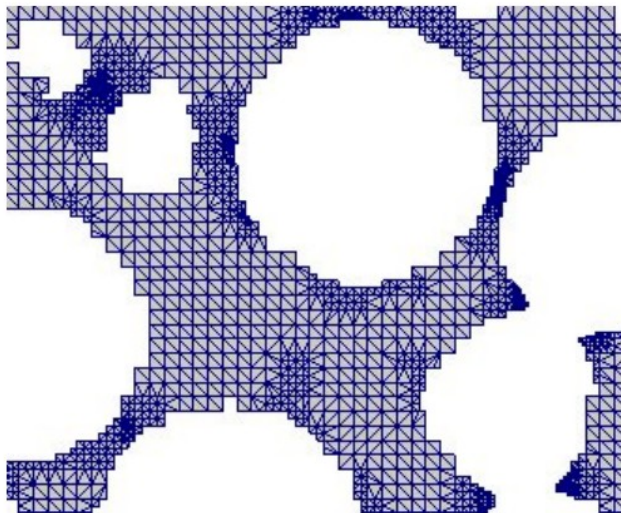
HPC center EOS-Calmip:
Typically: 10^8 mesh cells
 10^5 cores \times hours

} often
limited to
 $\sim \text{mm}^3$!



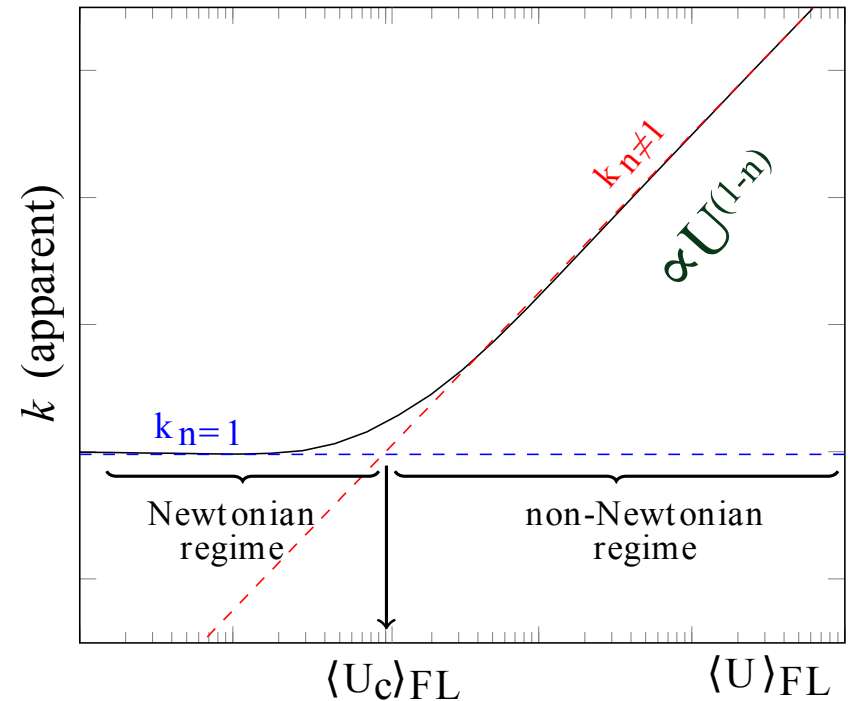
Resolution with OpenFoam

- FVM with OpenFOAM (SIMPLE, second-order scheme)
- Use of HPC, calculations up to 100 millions mesh elements
- a total of 100000 hours of CPU time.
- Conform orthogonal hexahedral elements.
- Multi-criteria grid convergence study = OK.



Results

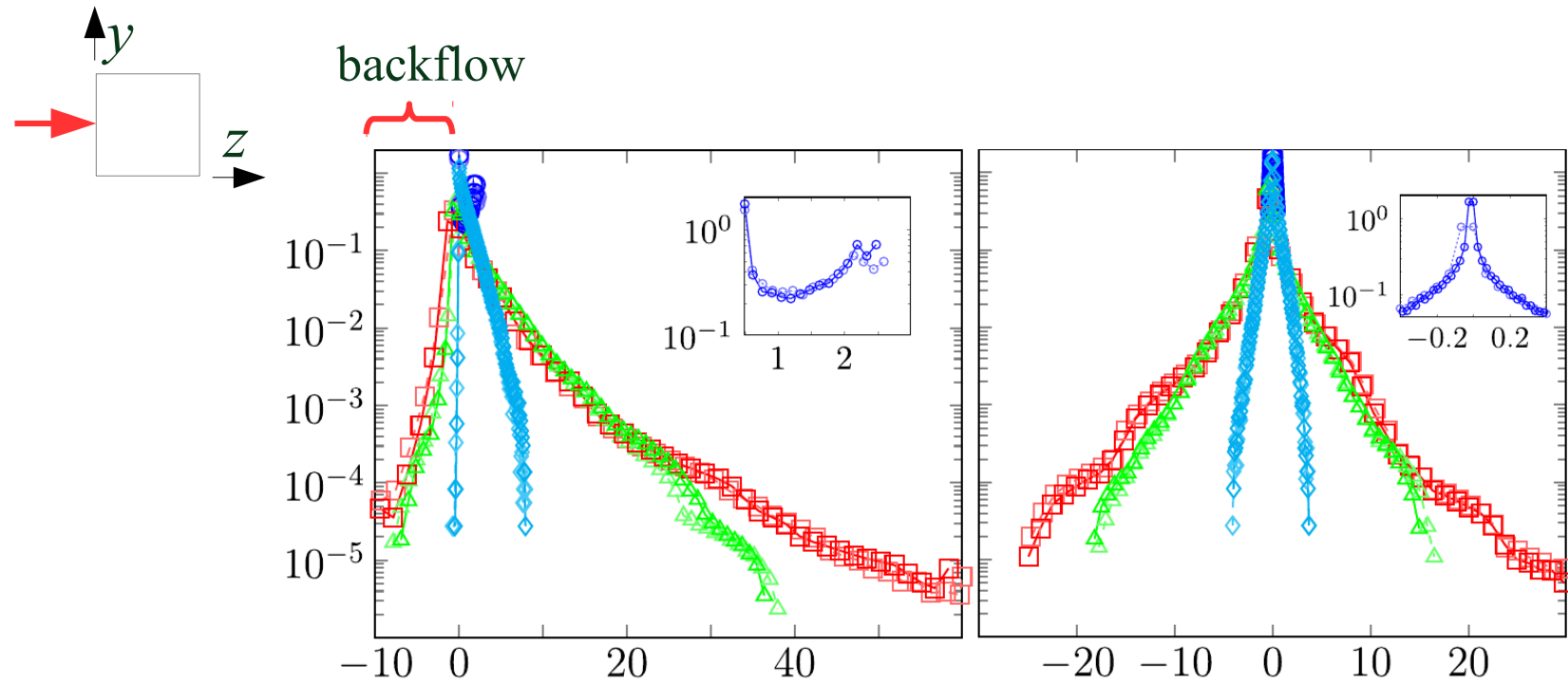
- Computations allows to analyze various features:
 - Properties of pore-scale fields (PDFs)
 - Transition:
 - Starts in a few narrow constrictions
 - Scaling for transition?



$\langle \cdot \rangle_{FL}$ = intrinsic fluid
average



Structure of the Velocity Field



newtonian

non-newtonian

(a) PDF of U_z^*

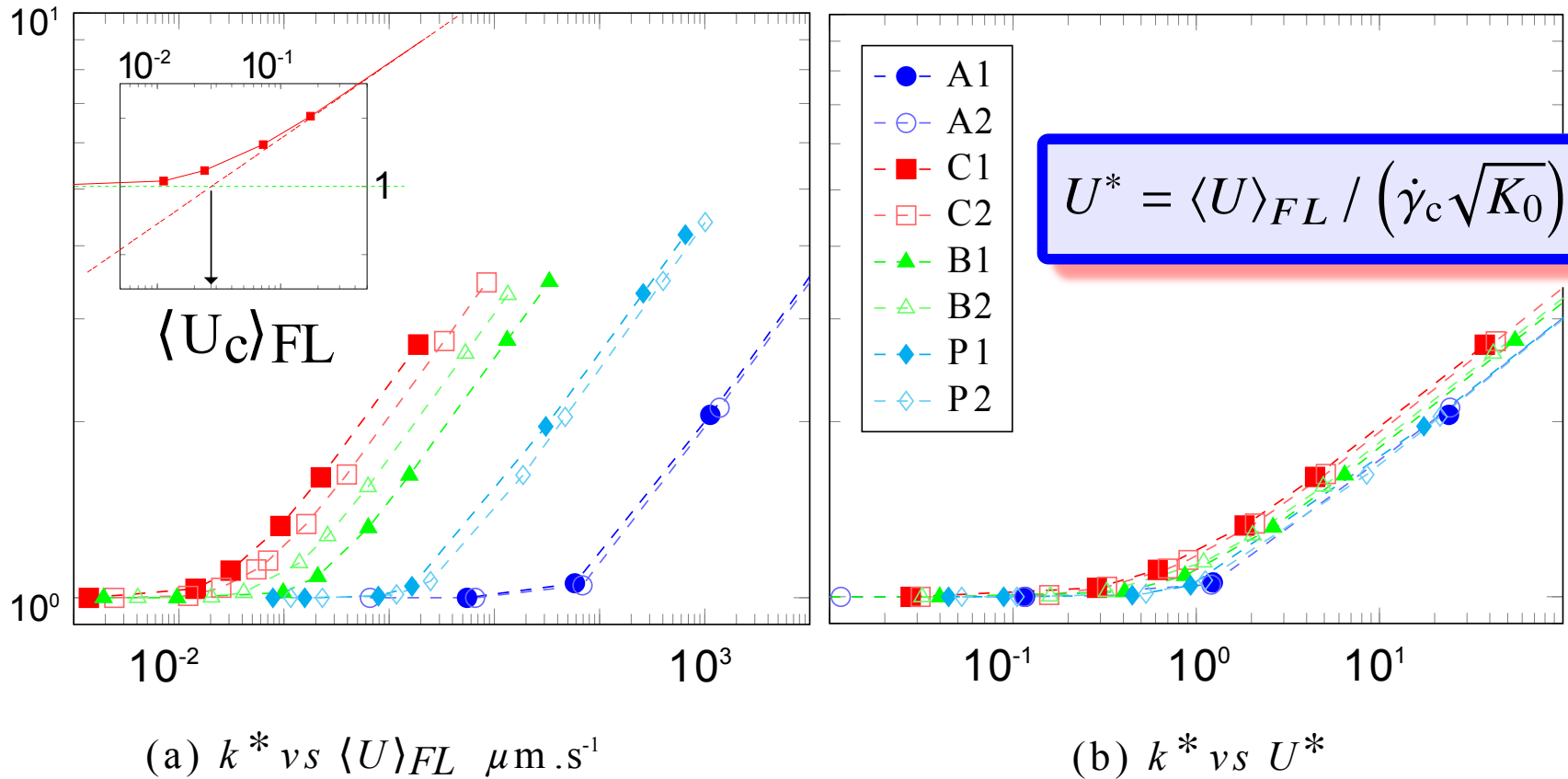
(b) PDF of U_y^*

- A2 $n = 1.00$ -△- B2 $n = 1.00$ -□- C2 $n = 1.00$ -◇- P1 $n = 1.00$
- A2 $n = 0.75$ -△- B2 $n = 0.75$ -□- C2 $n = 0.75$ -◇- P1 $n = 0.75$

Normalized pdf ~similar between Newtonian and non-Newtonian flow! Not valid for pdf of $\nabla\langle p_\beta \rangle^\beta$



Transition Scaling



$$\dot{\gamma}_c = 1\text{s}^{-1} ; n = 0.75$$

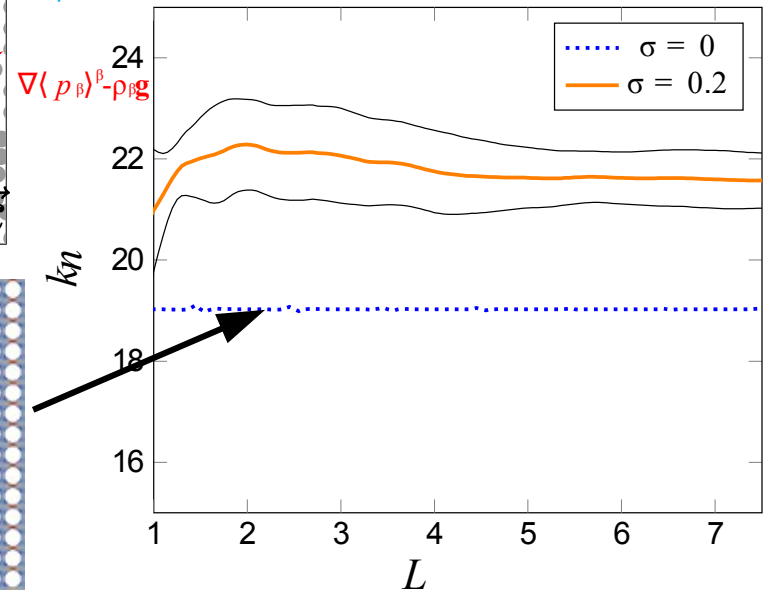
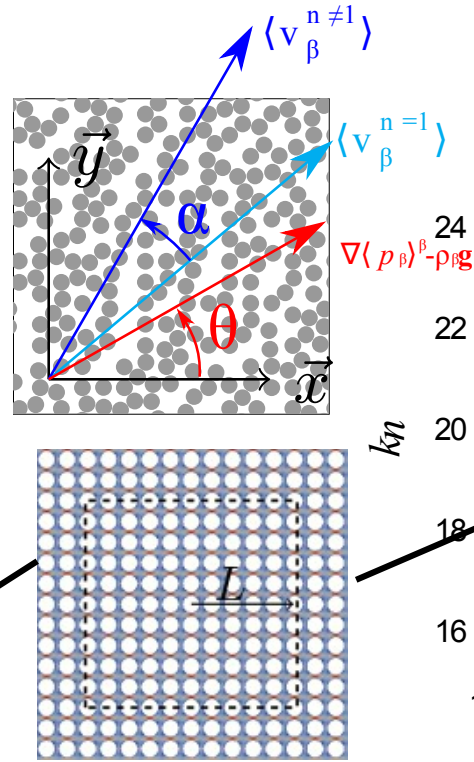
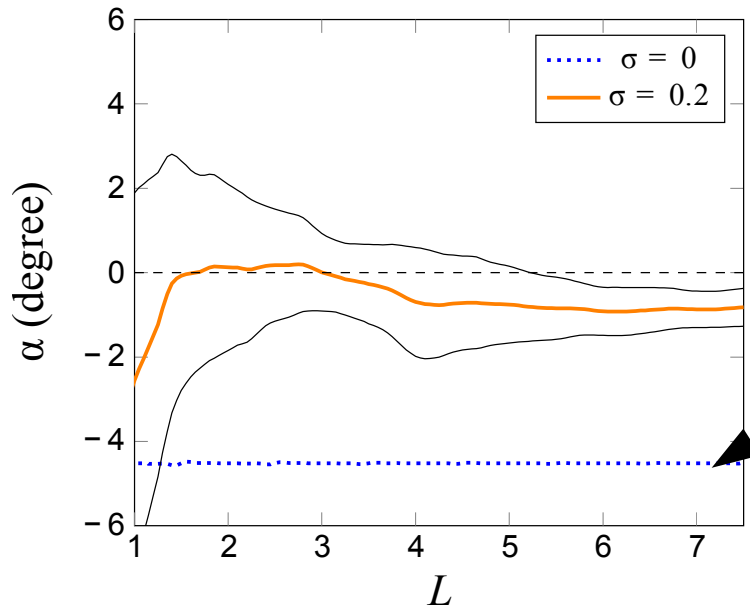
Zami-Pierre et al., 2015



Impact of Domain Size

$$\dot{\gamma}_c = 1 \text{ s}^{-1} ; n = 0.70$$

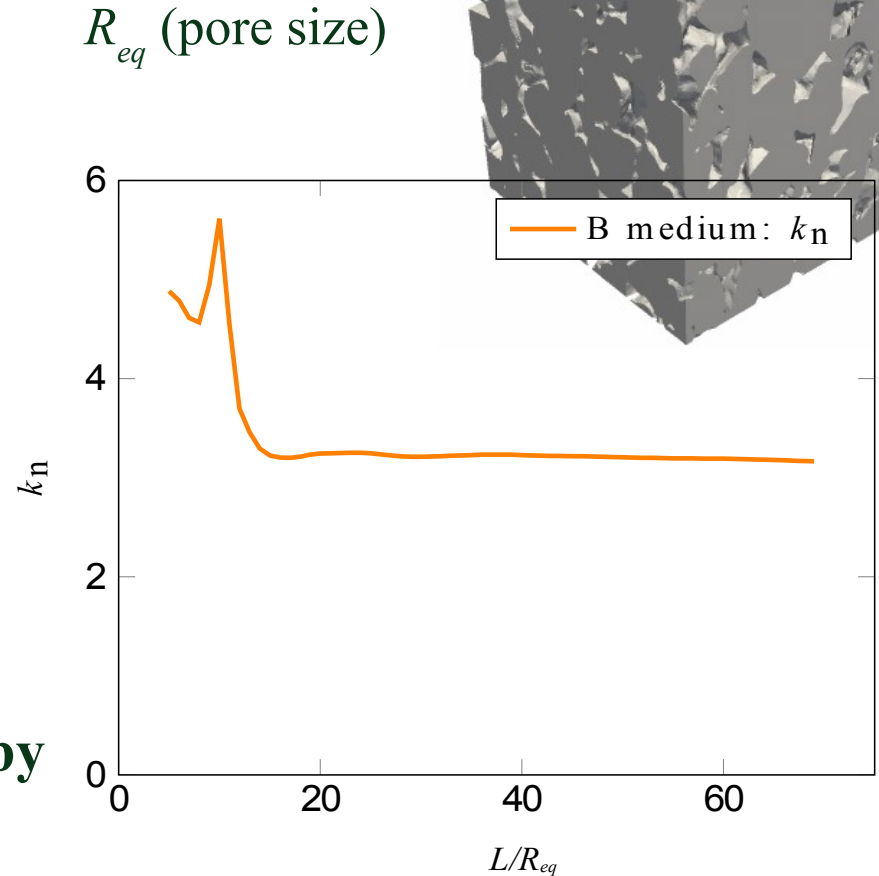
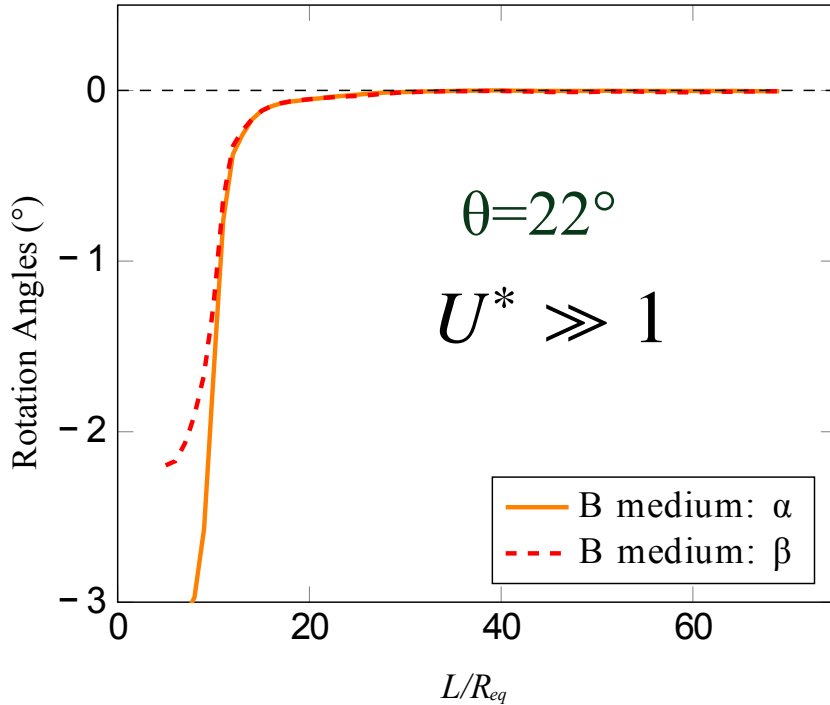
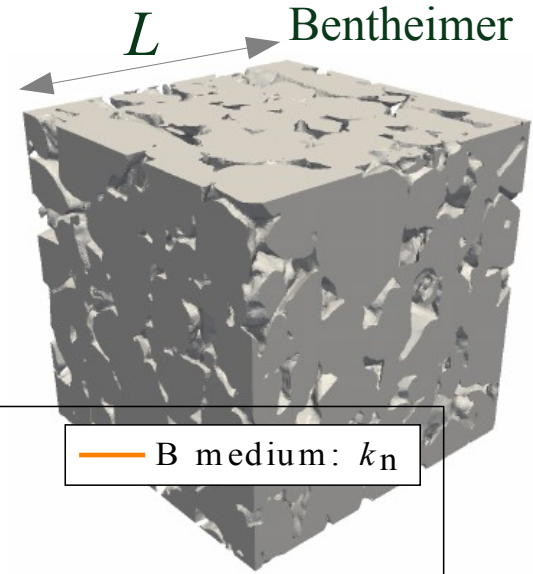
$$\theta = 22^\circ \quad U^* \gg 1$$



- Anisotropy induced by non-linear behavior decreases with $\nearrow L$ for disordered media
- Effective property variance decreases with $\nearrow L$



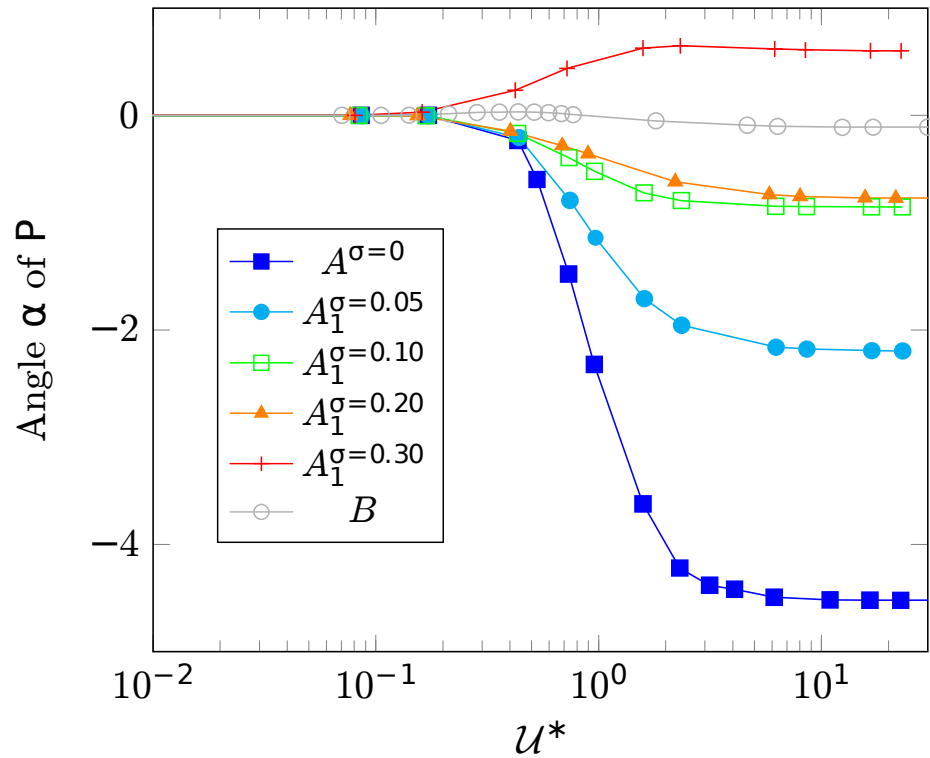
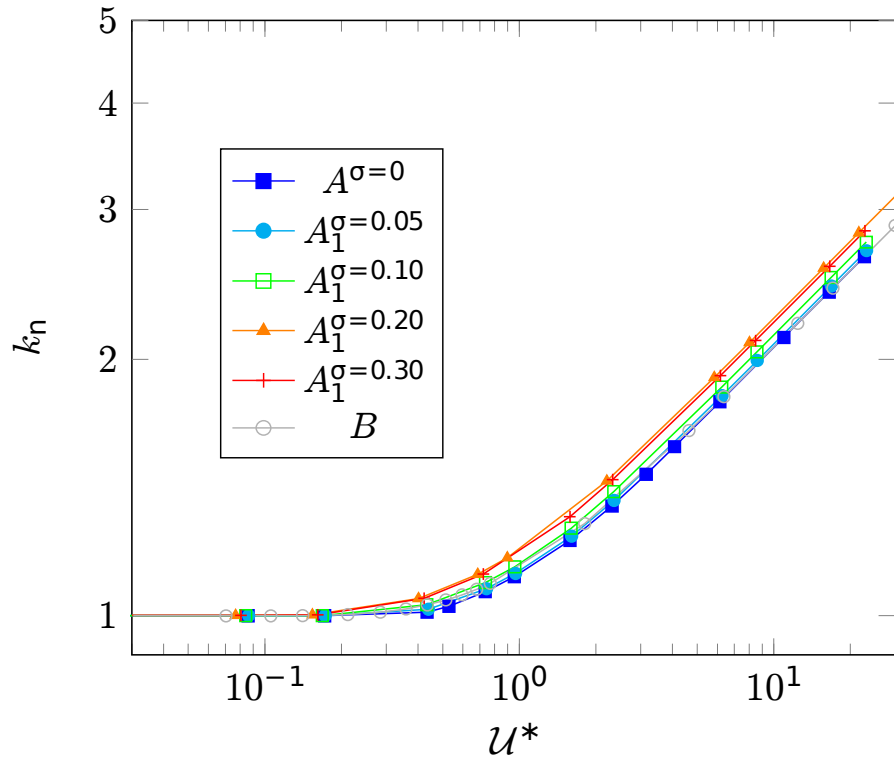
Impact of Domain Size



Disorder \rightarrow no anisotropy induced by non-linearity if L large enough!



Impact of disorder and velocity



Practical Consequences

- Eng. Practice: apparent Darcy's law

$$\langle \mathbf{v}_\beta \rangle = -\frac{1}{\mu(\dot{\gamma}_{eq})} \mathbf{K}_0 \cdot \left(\nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g} \right) \quad \dot{\gamma}_{eq} = 4\alpha \frac{\|\langle \mathbf{v}_\beta \rangle\| / \varepsilon_\beta}{\sqrt{8K_0 / \varepsilon_\beta}}$$

- Discussion:

Fitting parameter (rock dependent)

- P=I for all $\langle \mathbf{v}_\beta \rangle^\beta$ if isotropic disordered media and REV (\rightarrow **need tests for various sizes**)!
- Apparent permeability \sim scales with $(K_0)^{1/2} \rightarrow$ classical scaling “may” introduce artificial dependence upon parameters such as porosity:

$$\langle U_c \rangle_{FL} = \alpha' \dot{\gamma}_c \sqrt{K_0} \quad \text{VERSUS} \quad \langle U_c \rangle_{FL} = \frac{1}{\alpha \sqrt{2\varepsilon_\beta}} \dot{\gamma}_c \sqrt{K_0}$$

- Description of transition near the critical velocity may not be well described by an apparent viscosity (**no observed angle in the apparent permeability in the case of PLCO**)



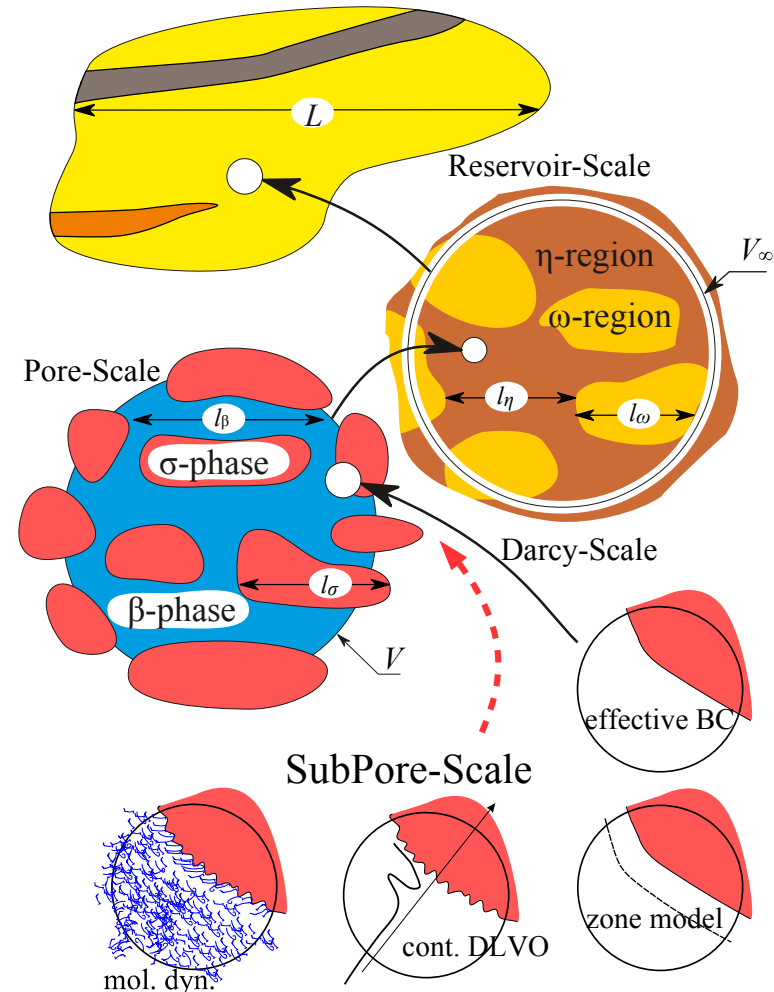
Further upscaling

- Depletion layer treated as an effective BC

$$\mathbf{v}_\beta = -\ell \mathbf{n} \cdot (\nabla \mathbf{v}_\beta + (\nabla \mathbf{v}_\beta)^T) \cdot (\mathbf{I} - \mathbf{nn})$$

Zami-Pierre et al., 2017

see Chauveteau (1982),
Sorbie & Huang (1991)
(double-layer model)



Further upscaling

- **Viscoelastic fluids**

$$\rho_l \frac{\partial \mathbf{v}_l}{\partial t} + \rho_l \mathbf{v}_l \cdot \nabla \mathbf{v}_l = -\nabla p_l + \rho_l \mathbf{g} + \underbrace{\nabla \cdot \left(\mu_s \left(\nabla \mathbf{v}_l + \nabla \mathbf{v}_l^T \right) \right)}_{\text{solvent}} + \nabla \cdot \boldsymbol{\tau}_v$$

$$\overset{\nabla}{\boldsymbol{\tau}}_v = \frac{\partial \boldsymbol{\tau}_v}{\partial t} + \mathbf{v}_l \cdot \nabla \boldsymbol{\tau}_v - \nabla \mathbf{v}_l^T \cdot \boldsymbol{\tau}_v - \boldsymbol{\tau}_v \cdot \nabla \mathbf{v}_l \quad \text{upper convected Derivative}$$

- **Rheological models**

FENE-P:

$$f(\boldsymbol{\tau}_v) \boldsymbol{\tau}_v + \lambda \overset{\nabla}{\boldsymbol{\tau}}_v = 2 a \mu_p \frac{1}{2} \left(\nabla \mathbf{v}_l + \nabla \mathbf{v}_l^T \right)$$
$$f(\boldsymbol{\tau}_v) = 1 + \frac{3 a + (\lambda/\mu_p) \text{tr}(\boldsymbol{\tau}_v)}{L^2} ; a = \frac{L^2}{L^2 - 3}$$

$L^2 \rightarrow \infty$ gives Oldroyd-B model (no-elongation limit)

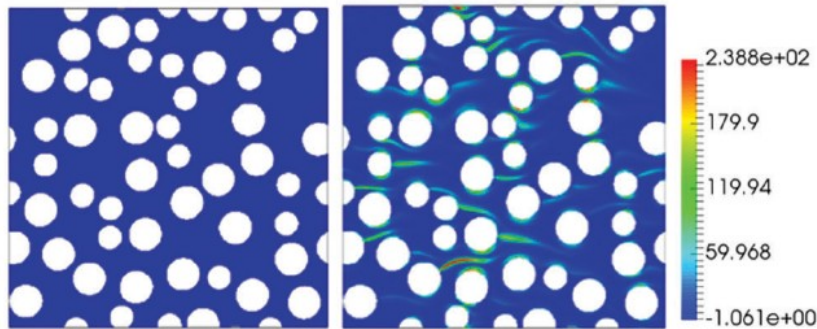


Example of results: De et al., soft matter, 2018

Steady-state!

Deborah number: $De = \frac{\lambda U_r}{L_r}$

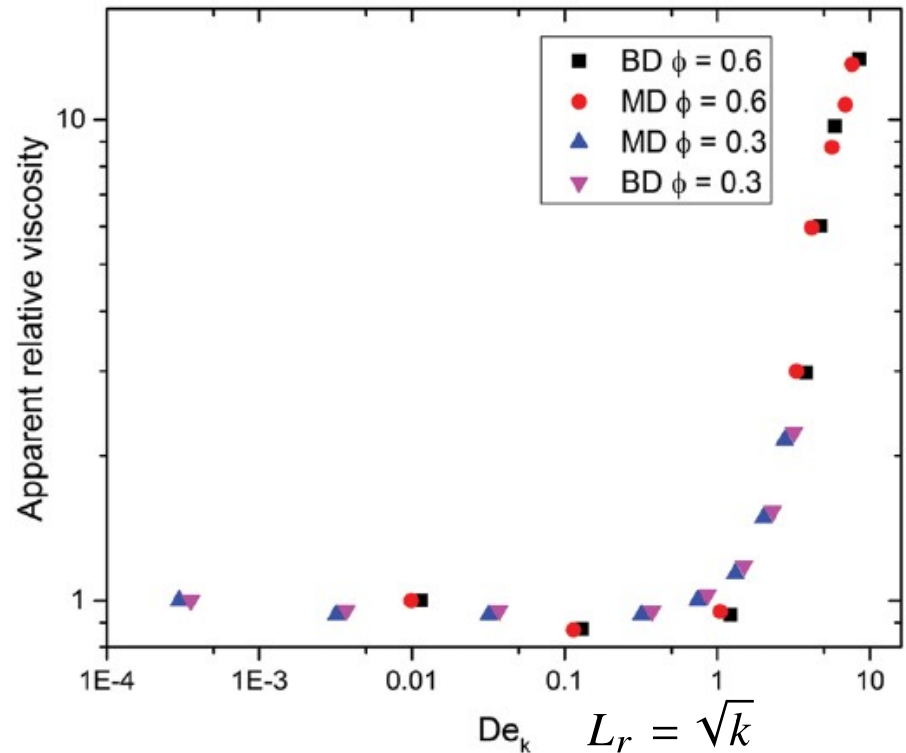
...also Weissenberg number ☺



De = 0.001

0.1

Normal stress along average flow
direction



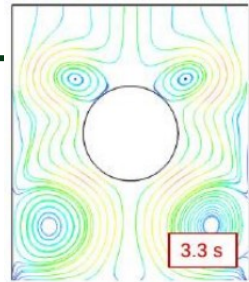
- see previous discussion on “apparent permeability”, etc...
- elastic turbulence?



Further perspectives: N-momentum equations, multi-component aspects, ...

- **Superfluid: 2 momentum equations → complex behavior → macro-scale model?**

see Allain et al. (2010, 2013, 2015), Soullaine et al. (2015, 2017)



- **Polymer solution as multi-component systems:**

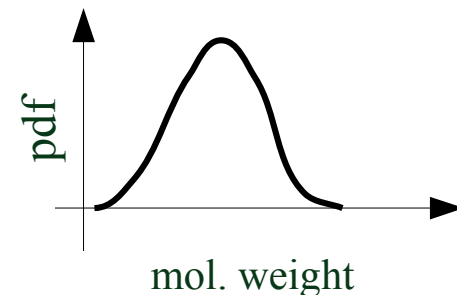
- Mechanical segregation, degradation (bio., mech.)
- Model?

- **Momentum balances:**

- diffusion theory or
- N-momentum equations

- **Composition:**

- Continuous models or
- PBM (population balance model), ...



Conclusions

- Upscaling tells that this is not always possible to separate in an apparent Darcy's law permeability and viscosity
- Specific anisotropy effects
- Simplifications arise for disordered media
- Various results published in the literature for various rheology: power-law (...), Ellis and Herschel–Bulkley fluids (Sochi & Blunt, 2008), Yield-Stress Fluids (Sochi, 2008), etc...
- Additional problems: retention effects, Inaccessible Pore Volume (IPV), mobile/immobile effects
- Perspectives: viscoelastic, multicomponent, coupling with other transport problems (transport of species, heat transfer, etc...), ...

