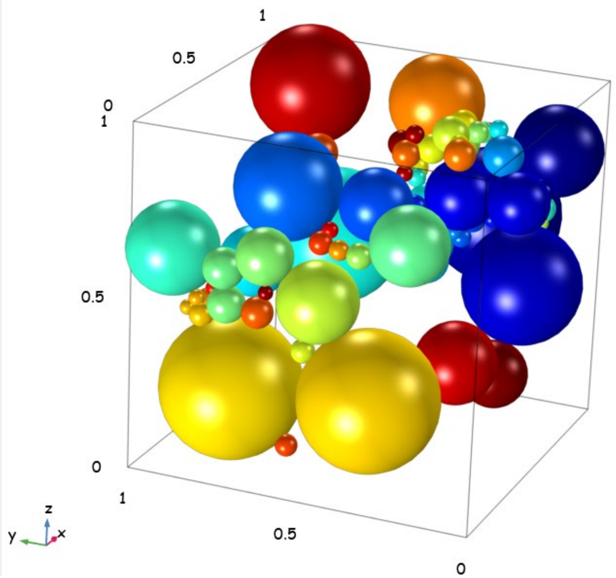
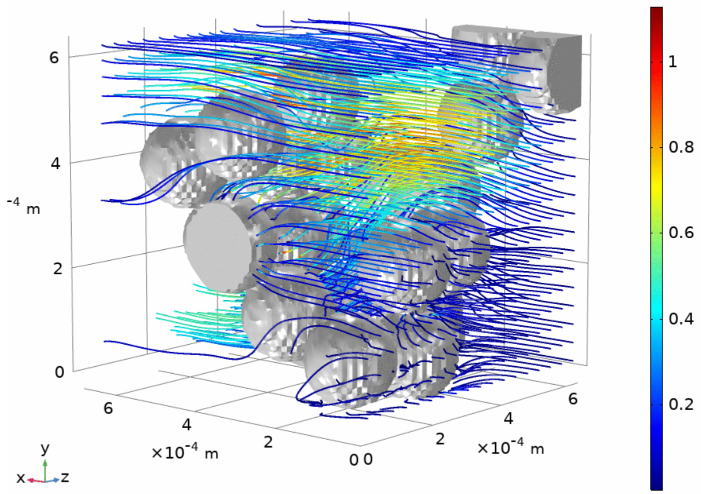


Microscopic and Macroscopic Modeling of Non-Isothermal Flow through Porous Media

October 25-27, 2023



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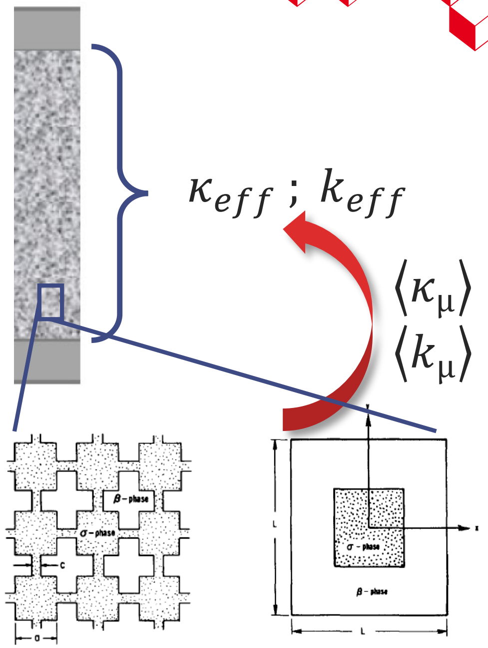
Introduction topics

∃ many analytical formulations for thermal and fluid effective properties (Mscale)

Coming from BCs hypothesis and averaging technics on elementary unit at µscale



Continuous or discontinuous σ phase [Nozad1985]

$$\kappa_{eff} = \frac{d_p^2}{cste} f_p(\epsilon)$$

Leading to fitting parameters to account for µscale specificities

$cste = 72, 150, 180$ *mainly from* τ

What is the specific relationship between effective macroscopic homogenous properties used in continuum equations and microstructure ?

Presentation Outline

1. Numerical Twins & Powder analysis : RVE generation
2. Modeling and Governing Equations : Fluid Flow/HT & Numerical aspects
3. Results and discussion : Effective Thermal Conductivity / Permeability
4. Summary and Outlook

1. Numerical Twins & Powder analysis

Numerical twin strategy

Powder analysis

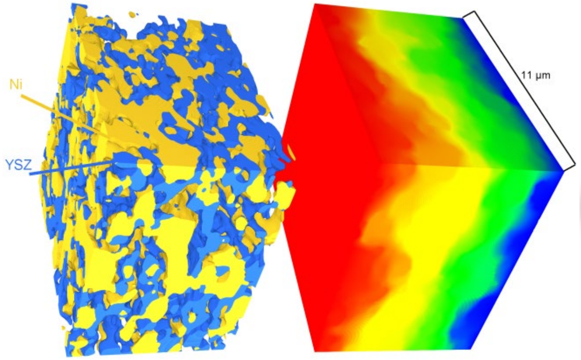
RVE generation

Strategies to have access to µstructure

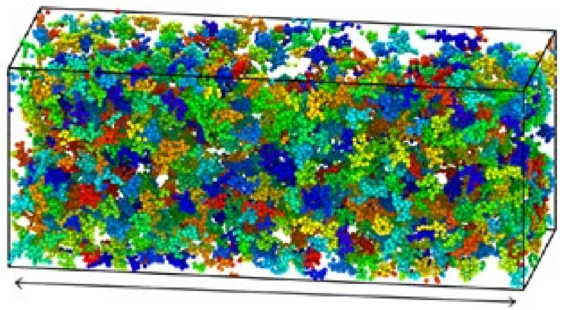
- From real microstructure approach (not developed)
  - 2D SEM with different slices
  - 3D tomography
  - Reconstruction and numerical transfer to FEM code (sometimes laborious with manual cleaning and filtering)

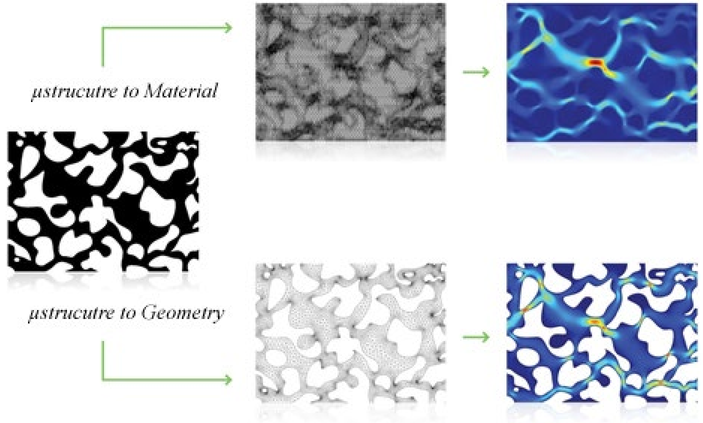
- From statistically Representative Volume Element (RVE) with microstructural information (SSA, ϵ…)
  - Numerical twins
  - Homemade software for particles microstructure generation (genefrac)

- Front Tracking method (microstructure to geometry) vs Front Capturing method (microstructure to material)
  - Material properties following microstructure
  - FC method efficiency (computational cost)
  - FC versatile method (coarsening or refining mesh)



3D reconstructed SOFC anode
Electric field in the porous media
[VIVET2011]

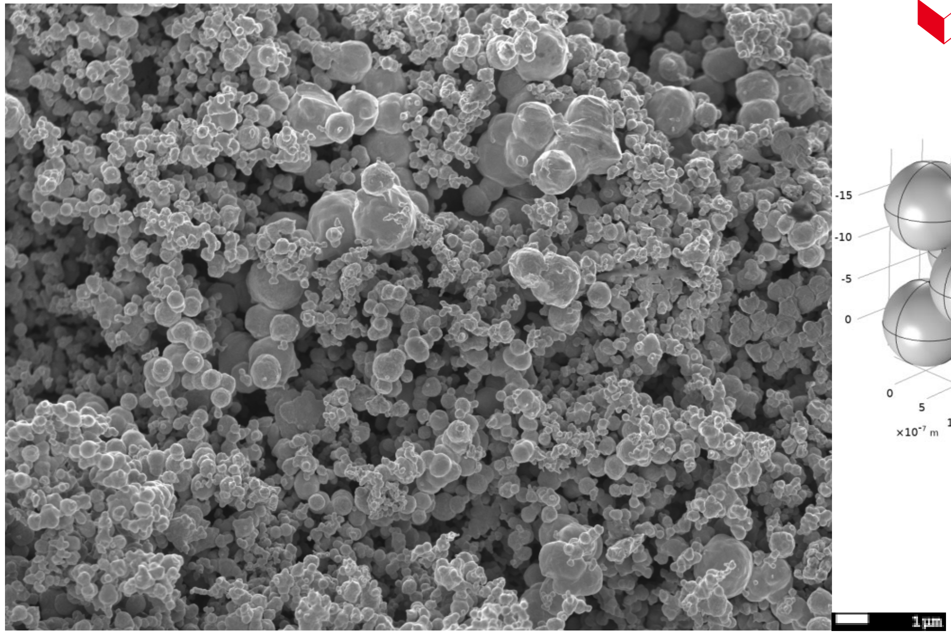

[GUESNET2018]

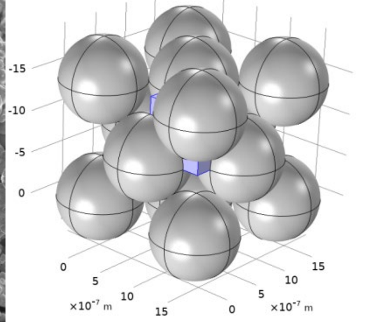


[COMSOL2017]

Powder analysis

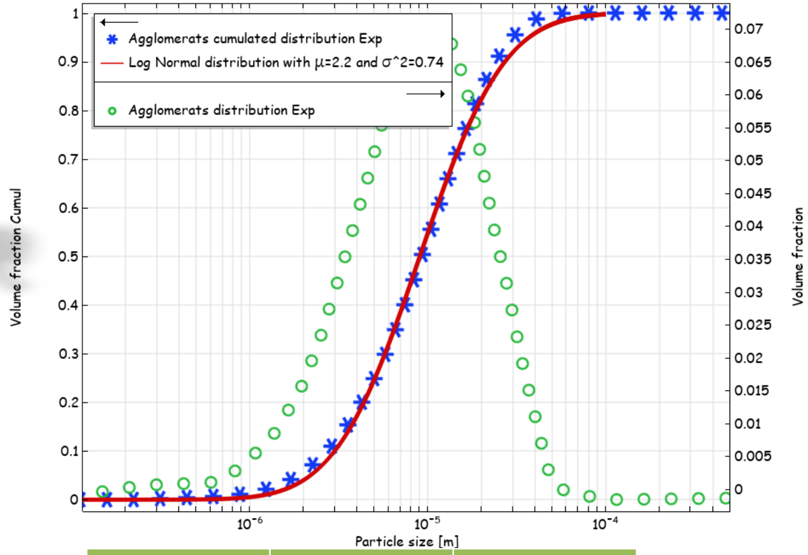
- Ideal sphere hypothesis usually used
  - SSA measured by BET technique $\approx 1[m^2/g]$
  - $S_0 = \frac{6}{d_{eq}}$ gives an equivalent diameter
  - $d_{eq} \approx 500[\text{nm}]$ consistent with SEM observations





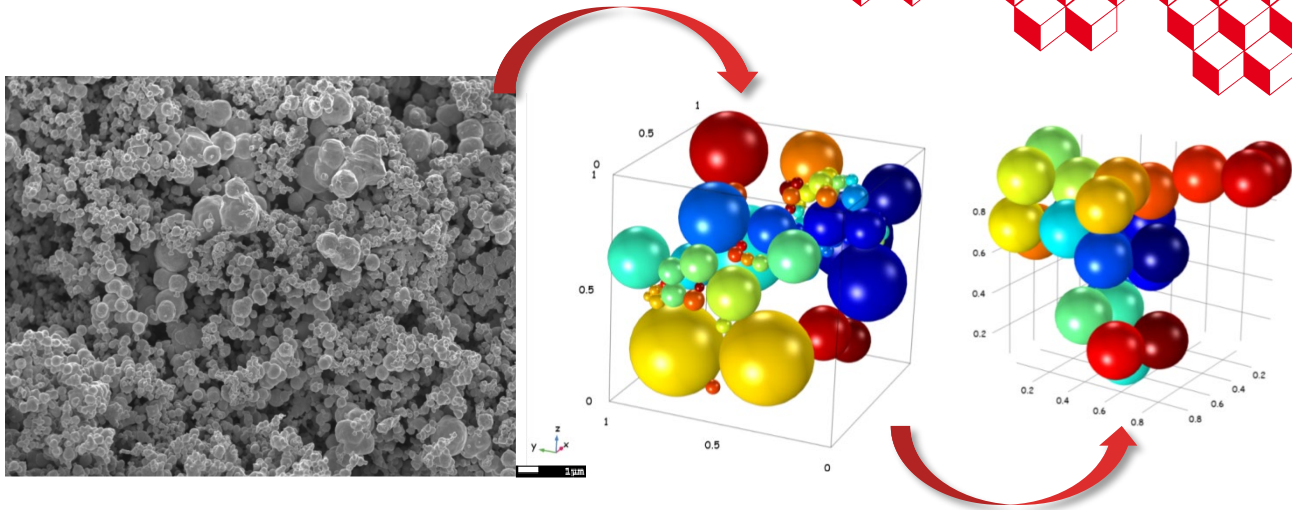
- But
  - It's all but a simple crystallographic organization
  - a bimodal distribution is observed
  - Particles are not so spherical

- Consequently, porosity (Volumetric density measurement) is higher than the ideal crystallographic organization
  - Agglomerates of about 10[µm] characterized by laser particle size analysis

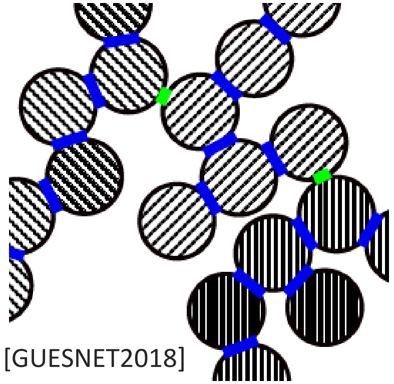


d_{10}	d_{50}	d_{90}
2.7 µm (1) RSD = 8.7 %	9.3 µm (1) RSD = 6.0 %	24.1 µm (1) RSD = 8.1 %

RVE generation
genefrac [ROCHAIS2022]

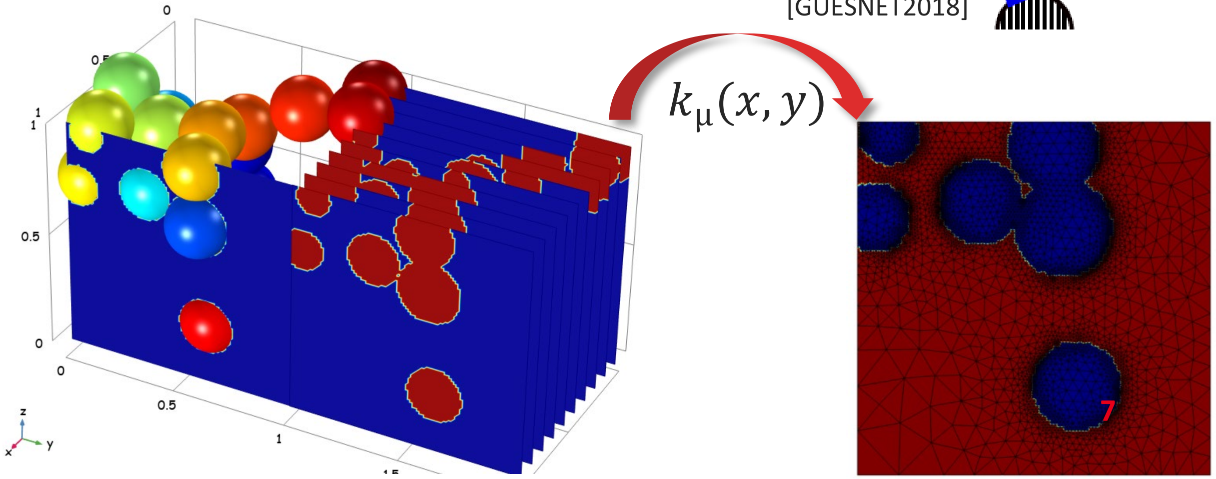


- µstructure generation with physical characteristics from homemade software Genefrac
- Simplified to
  - 26 particles of 400[nm] diameter and 50[nm] overlap ϵ 0.75 and SSA 1.17[m²/g]
  - 3 agglomerates
    - particles connections for continuous σ phase(blue) but unconsolidated material
    - Consolidated material with additional hertz contact (green)



[GUESNET2018]

- 2D calculations with 11 slices to reduce 3D computational cost
- Front Capturing method with microstructure to material approach and mesh refinement
  - Spatial dependency of local physical props



2. Modeling and Governing Equations

Fluid flow and HT

Numerical aspects

Modeling and Governing Equations
Fluid flow and HT

- HT at Mscale
  - Heat equation for stationary conditions
    - $\nabla \cdot \left(-k_{eff}\ \nabla T\right) = 0$
  - Effective conductivity at Mscale from analytical formulations

- HT at µscale
  - Heat equation for stationary conditions
    - $\nabla \cdot \left(-k_{phase} \nabla T\right) = 0$
  - Each local material properties are spatial functions of the µstructure distribution wo geometrically defined domains
    - $k_{phase} = k_s f_s + k_f (1 - f_s)$
  - Effective conductivity from µscale calculation
    - $k_{eq} = \frac{\iint -k \nabla T d\Gamma_{in}}{(T_{out} - T_{in}) L}$

$k_{eff} = \varepsilon k_f + (1-\varepsilon) k_s$

Volume Avg/Arithmetic mean/Parallel distribution

$k_{eff} = 1/(\varepsilon / k_f + (1-\varepsilon)/k_s)$

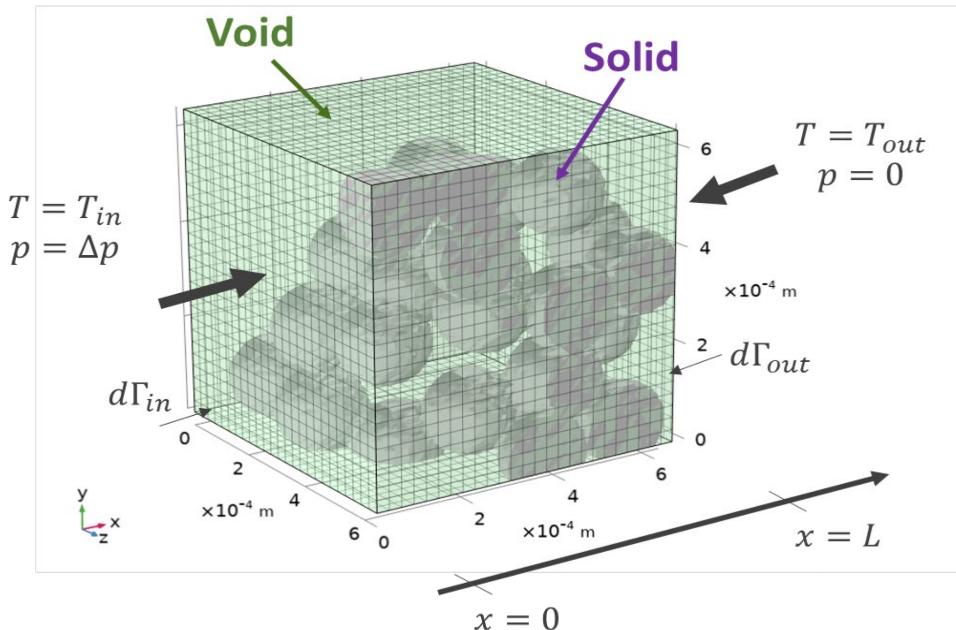
Reciprocal Avg/Harmonic mean/Series distribution

$k_{eff} = k_f^{\varepsilon} . k_s^{(1-\varepsilon)}$

Power Law/Geometrical mean/Random distribution

$k_{eff} = k_f . \left(\varepsilon + \frac{(1-\varepsilon)}{\left(0.22\varepsilon^2 + \frac{2k_f}{3k_s}\right)} \right)$

[Kunii1960]



Modeling and Governing Equations
Fluid flow and HT

- Fluid Flow at Mscale
  - Darcy's law, mass conservation and Stationary conditions
    - $\nabla \cdot (\rho \boldsymbol{u}) = 0$
    - $\boldsymbol{u} = -\frac{\kappa}{\mu} \nabla p$
    - Darcy's velocity $u \neq \langle v \rangle$ the mean interstitial velocity

- Fluid Flow at µscale
  - Laminar flow (inertial terms) and Stationary conditions
  - Navier Stokes equations for mass and momentum balance
    - $\nabla \cdot (\rho \boldsymbol{v}) = 0$
    - $\rho \left(\boldsymbol{v} \cdot \nabla \right) \boldsymbol{v} = \nabla \cdot \left[-pI + \boldsymbol{K} \right] + \boldsymbol{F}$
    - Viscous stress tensor $K = \mu(\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^T)$
    - Volume drag force $\boldsymbol{F} = -K_{num}(x, y, z) * \boldsymbol{v}$
  - Effective permeability from µscale calculation
    - $\kappa_{eq} = \frac{\eta \bar{v} \varepsilon L}{\Delta p}$

$\kappa_{Kozeny} = \frac{d_{grain}^2}{180} \frac{\varepsilon^3}{(1-\varepsilon)^2}$

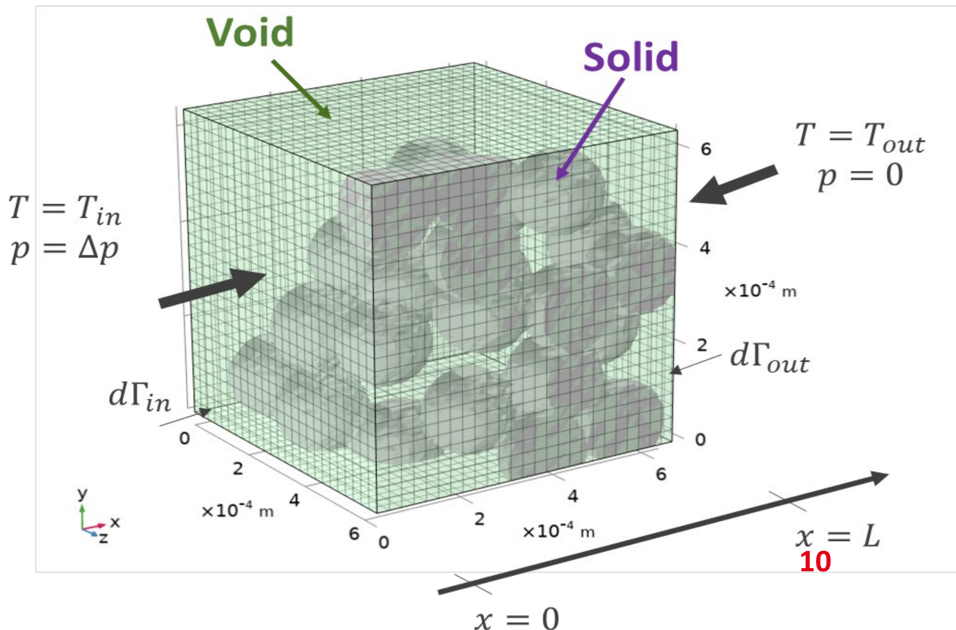
"conduit flow" with fitting constant for τ

$\kappa_{Brinkman} = \frac{d_{grain}^2}{72} \left(3 + \frac{4}{(1-\varepsilon)} - 3. \sqrt{\frac{8}{(1-\varepsilon)} - 3} \right)$

"flow around submerged objects"

$\kappa_{stokes} = \frac{2 d_{grain}^2}{36.(1-\epsilon)}$

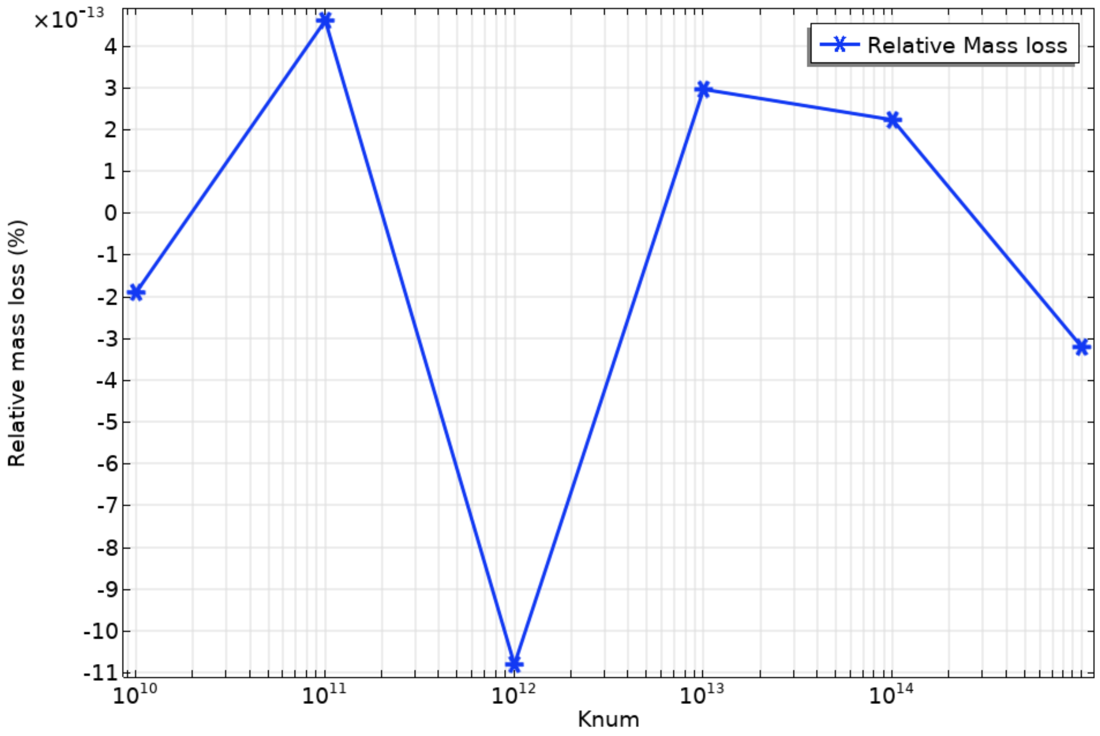
"flow around submerged objects" for limiting condition $\epsilon \to 1$



Modeling and Governing Equations
Numerical validations

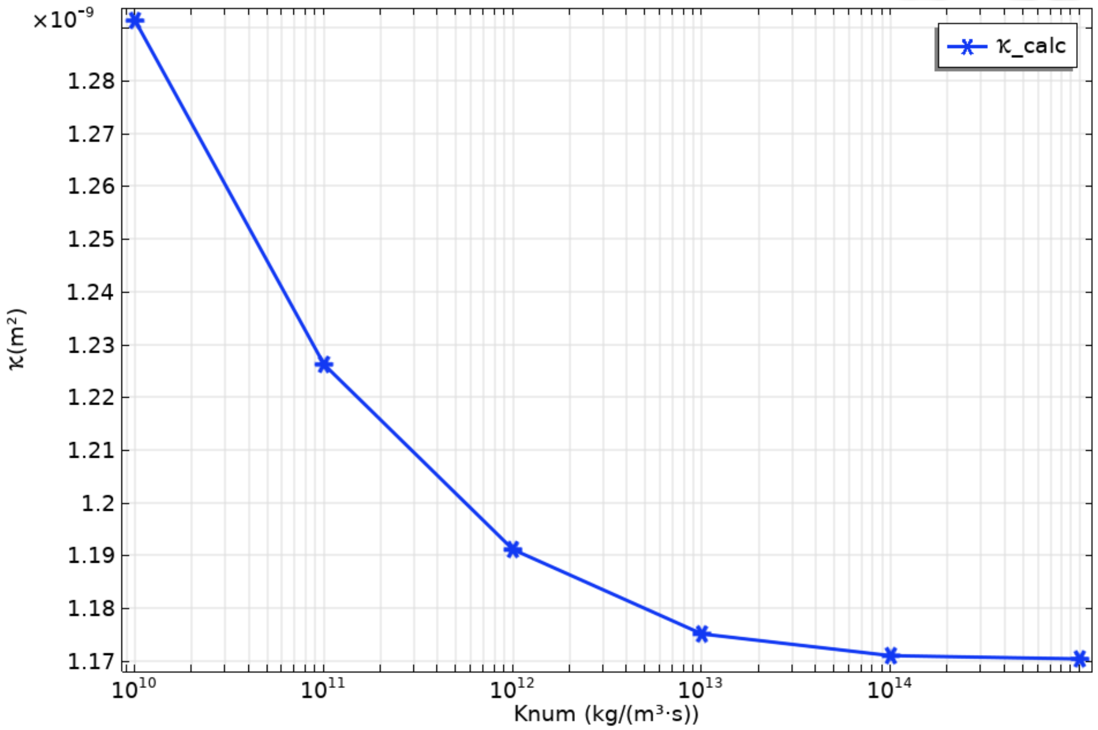
Numerical validation from mass conservation

Relative error is very low (below $\approx 10^{-12}$ %) **for each** K_{num}



Volume drag force influence on $\boldsymbol{\kappa_{eq}}$

Results independence for $K_{num} > 10^{14}$

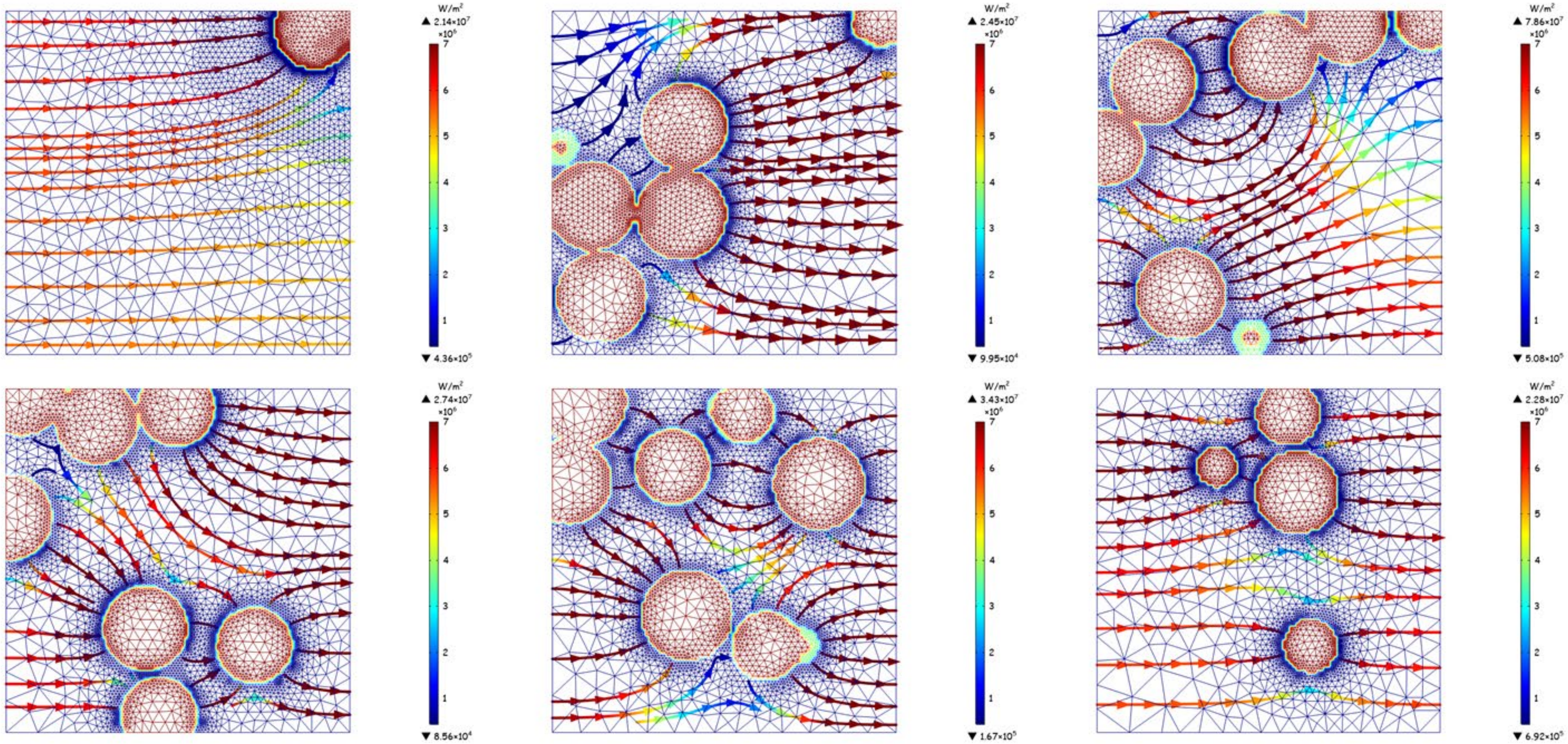


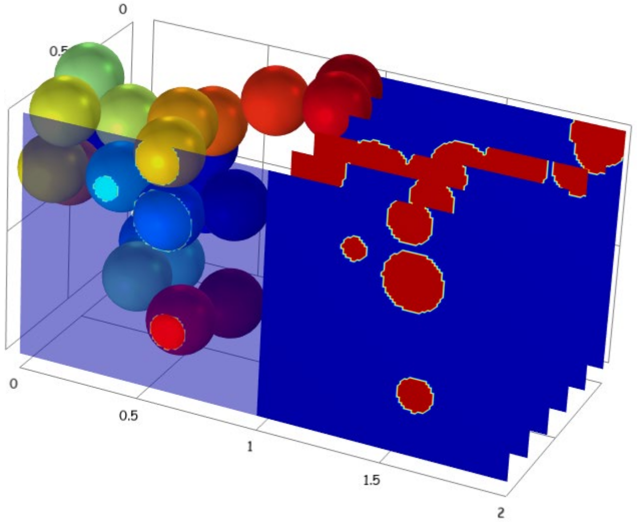
3. Results and discussion

HT / Effective Thermal Conductivity

Fluid flow / Effective Permeability

Results and discussion
HT / Effective Thermal Conductivity

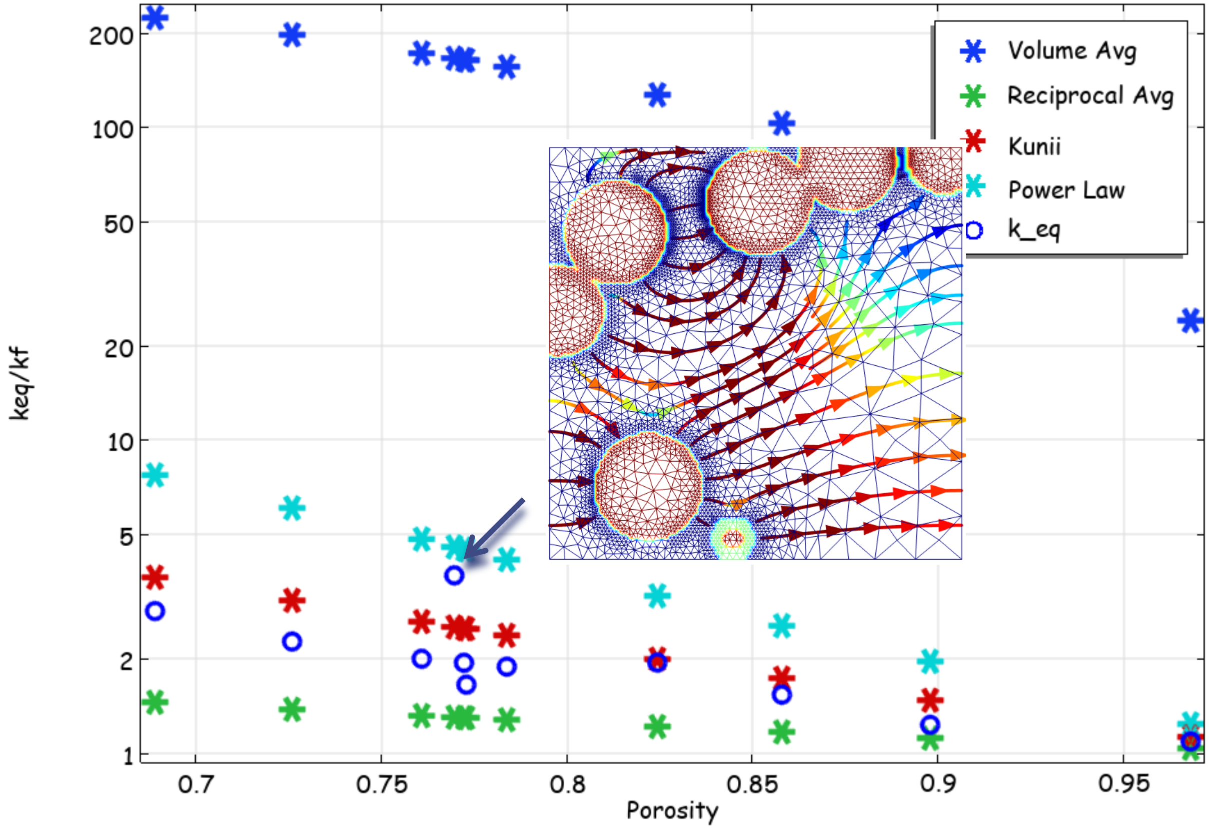


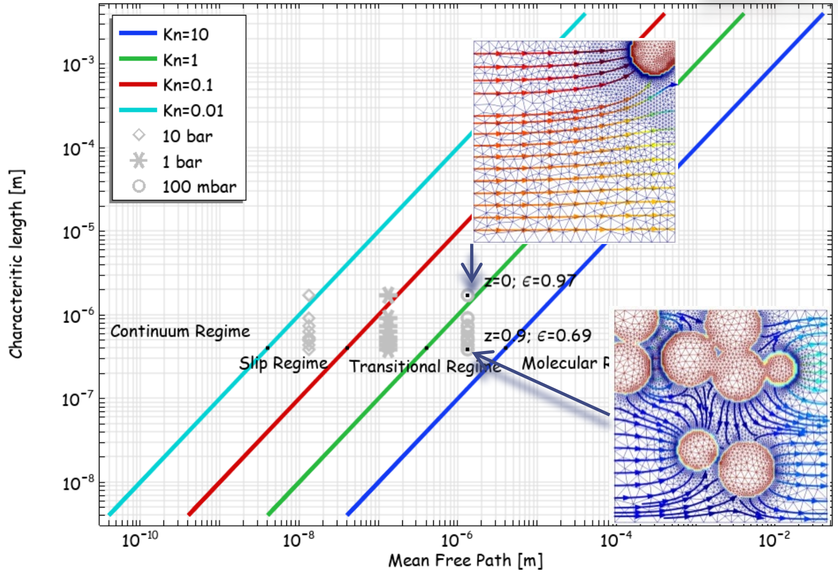


Each slice are calculated for 2D stationary cases with remeshing and heat flux influenced by :

- the relative magnitude of k_s/k_f (the same for each cases)
- the µstructure
  - continuity of solid phase and average porosity

Results and discussion
HT / Effective Thermal Conductivity





Degree of rarefaction : $K_n = \frac{\lambda}{C}$
(with C as a function of ϵ_{eq})

$0.01 < K_n < 0.1$
Slip regime

$0.1 < K_n < 10$
Transitional regime

$10 < K_n$
Molecular regime

$k_{eff} = \varepsilon k_f + (1-\varepsilon)k_s$
Volume Avg/Arithmetic mean/Parallel distribution

$k_{eff} = 1/(\varepsilon/k_f + (1-\varepsilon)/k_s)$
Reciprocal Avg/Harmonic mean/Series distribution

$k_{eff} = k_f^{\varepsilon}.\, k_s^{(1-\varepsilon)}$
Power Law/Geometrical mean/Random distribution

$$k_{eff} = k_f.\left(\varepsilon + \frac{(1-\varepsilon)}{\left(0.22\varepsilon^2 + \frac{2k_f}{3k_s}\right)}\right)$$

[Kunii1960]

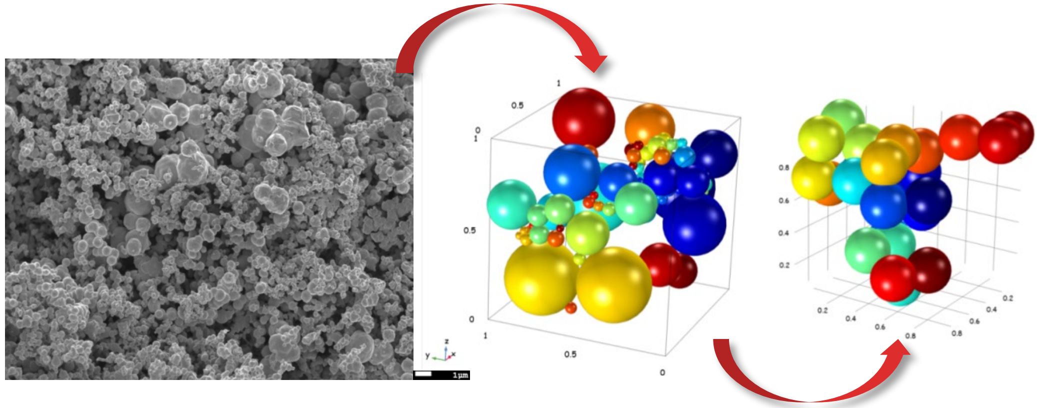
k_{eq} for numerical twin calculations is :

- close to the Kunii model, 2 decades lower than // distribution (by default) !! (highly insulated porous medium)
- Consistent with literature data for “high p – low ϵ – unconsolidated” material
- still under investigation for transition to molecular regime – high ϵ – consolidated

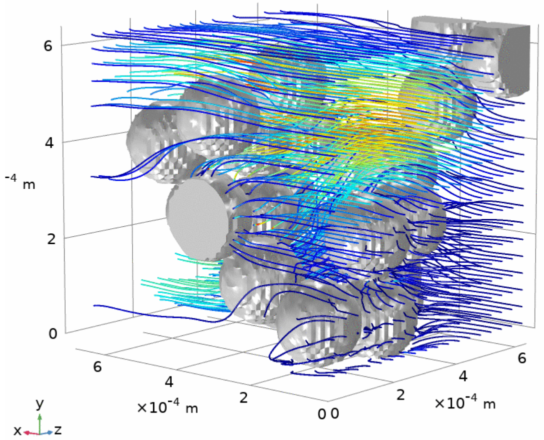
4. Summary and Outlook

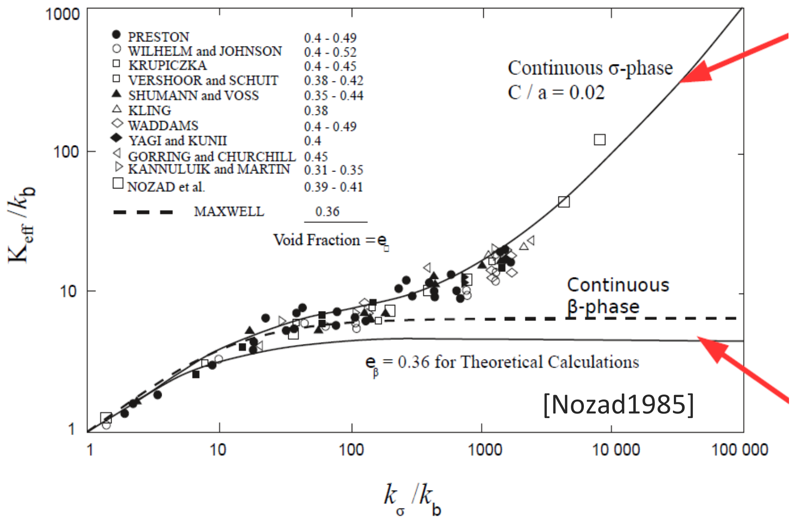
Summary and Outlook

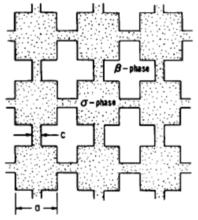
- Numerical twin strategy linking a homemade software for microstructure generation of consolidated particles with COMSOL Multiphysics® has been proposed
  - Could be an efficient tool to choose the right effective model at Mscale for thermal and fluid effective properties

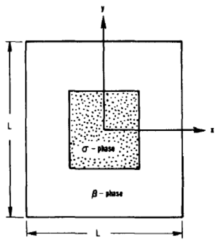


- Many interesting prospects are
  - BCs and RVE statistics
    - Calculation on larger number of particles
  - Study of specific µstructure influence on the effective response
    - anisotropy, bimodale distribution, degree of consolidation…
  - Study of particular regime for HT and Fluid flow for a wide range effective properties evaluation
    - Molecular regime, local chocked flow & turbulence effects
  - Physic's coupling
    - HT and flow coupling
    - Study of potential Local thermal non equilibrium
  - High order dimension
    - 3D simulation influence









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Thank you for your attention

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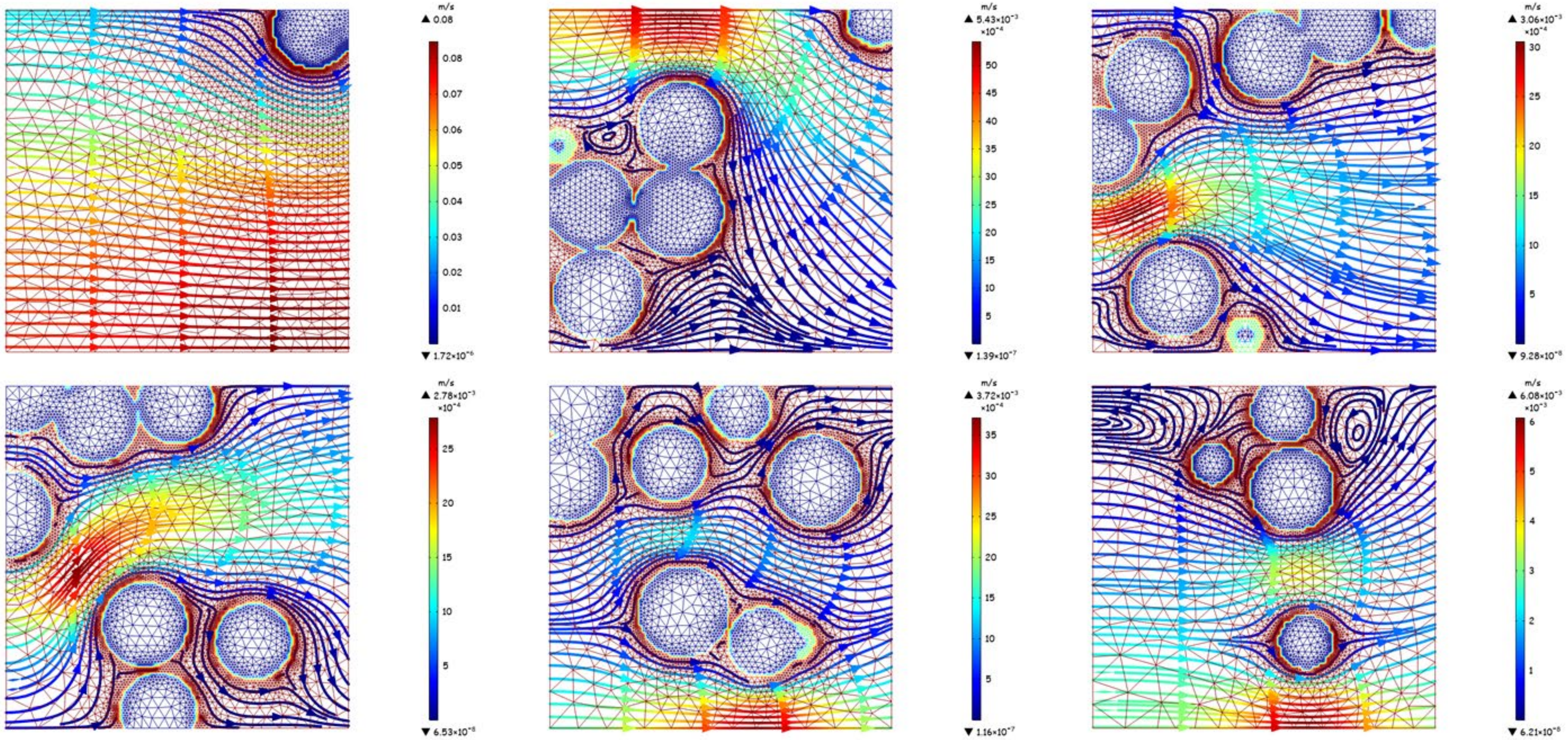
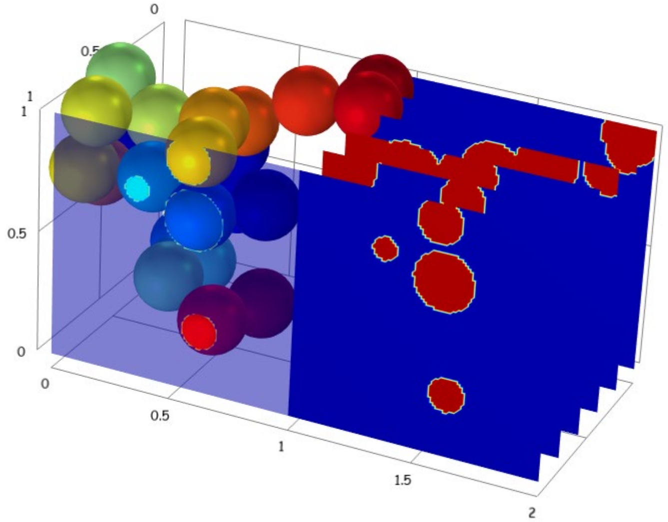
5. Back Up Fluid Flow

Results and discussion
Fluid flow / Effective Permeability

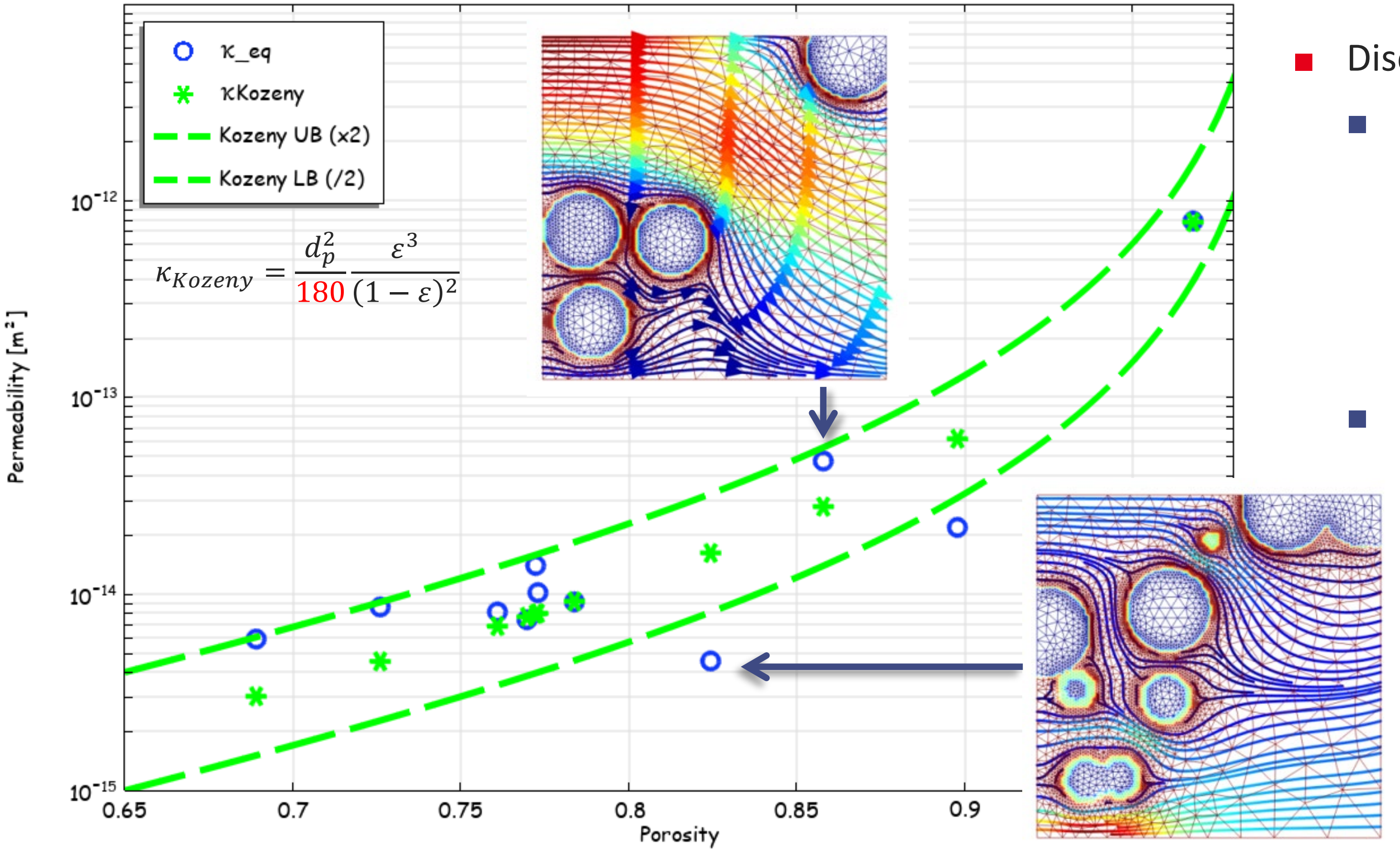




Each slice are calculated for 2D stationary cases with remeshing and laminar flow :

- Low velocity for this imposed ∇p
- Consistent with equivalent Mscale calculation for Darcian flow
- Local eddies depending on µstructure

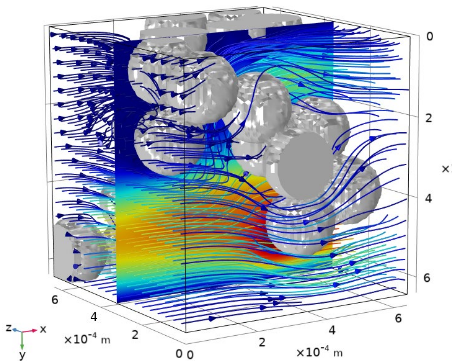
Results and discussion
Fluid flow / Effective Permeability

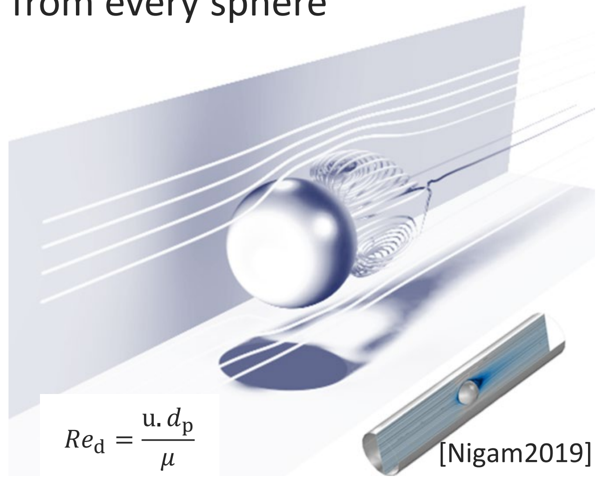


Effective permeability κ_{eq} ,calculated by numerical twin, exhibits :

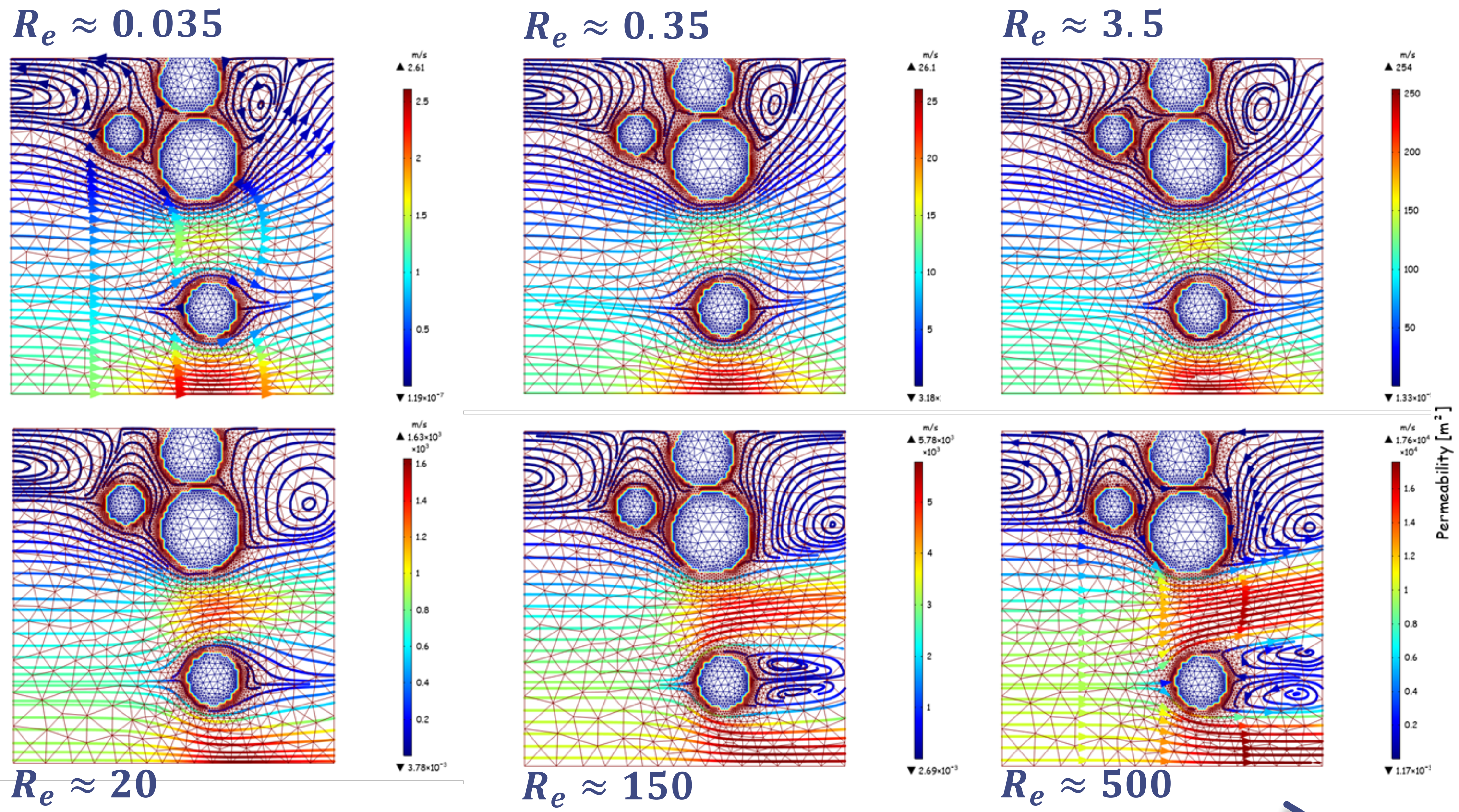
- Results close to κ_{Kozeny}
- A wide variability depending on local µstructure (channeling vs tortuosity effect)

- Discussion
  - κ_{Kozeny} based on the assumption of conduit flow with fitting constant for τ effect
    - Hypothesis should break down at high ϵ_{eff}
    - "flow around submerged objects" should be better at high ϵ_{eff}
  - BC's & dimension influence
    - The flow gets around the particle in 3D and 2D simulation could be too restrictive
    - the proximity of other spheres should influence wake formation downstream from every sphere

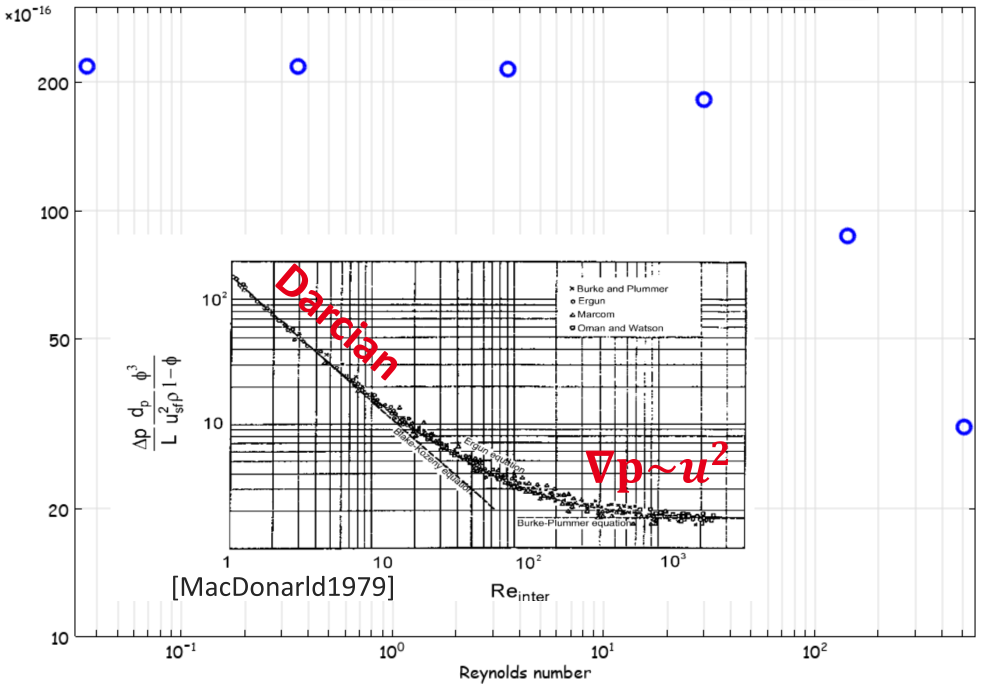




Results and discussion
Fluid Flow Regimes



Increasing ∇p & Re



Correlated at Mscale using Ergun equation for deviation of the Darcy's law for high Re & strong inertia (Non Darcian Flow)

$$\nabla p = -\frac{\mu}{\kappa}\boldsymbol{u} - \beta\,\rho|\boldsymbol{u}|\boldsymbol{u} \text{ with } \beta = \frac{c_F}{\sqrt{\kappa}}$$

$$\beta = \frac{1.75}{d_p}\frac{(1-\varepsilon)}{\varepsilon^3} \qquad \kappa_{Ergun} = \frac{d_p^2}{150}\frac{\varepsilon^3}{(1-\varepsilon)^2}$$

Local eddies starts to develop with increasing Re (>10)

- By increasing Re the flow regime gradually changes from laminar to turbulent
- Weak inertia regime consistent with literature 10<Re<100
- Inertial terms create additional pressure drop at high Re