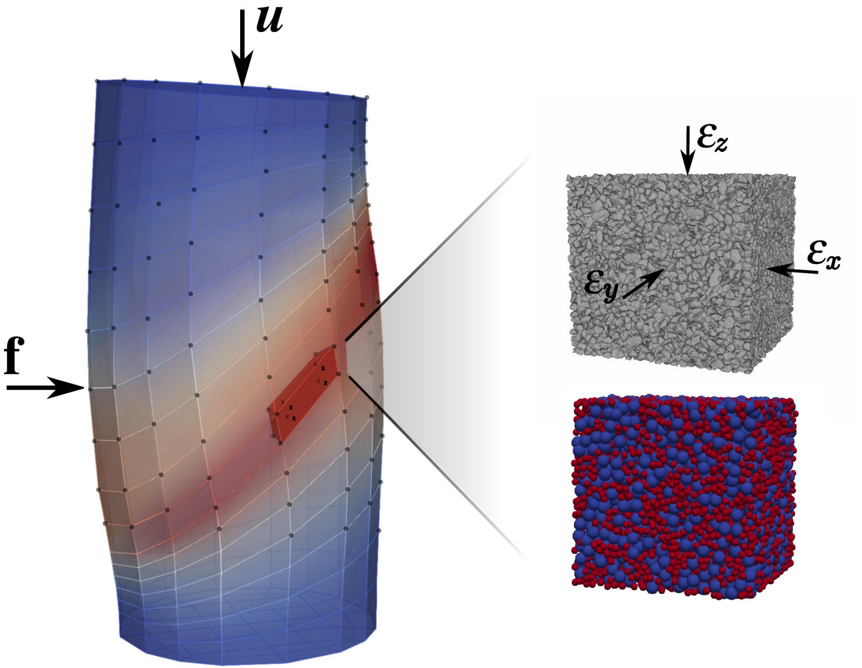

CIVIL-408 Multiscale Modeling in Mechanics

Prof. Kostas Karapiperis

Week 12

Quiz

Which of the following are true regarding multiscale modeling of fracture? Select all that apply.

a. We can use standard computational homogenization.

b. We can use non-standard computational homogenization ensuring energy consistency and kinematic enrichments at the macroscale.

c. We can use horizontal scale-bridging.

Quiz

Which of the following are true regarding multiscale modeling of fracture? Select all that apply.

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c. We can use horizontal scale-bridging.

Homogenization in multiphysics problems

- Poromechanics
- Heat conduction
- Thermoporomechanics
- Chemomechanics

Homogenization in multiphysics problems

- Poromechanics
- Heat conduction
- Thermoporomechanics
- Chemomechanics

Homogenization for poromechanics

Rocks

Microscale:
Fully resolved pore-scale fluid simulations using a kinetic-theoretic approach (LBM)

$$\frac{\partial f_i}{\partial t} + \boldsymbol{e}_i \cdot \boldsymbol{\nabla} f_i = C_i$$

↑ Particle distribution

Hill-Mandel

⟷

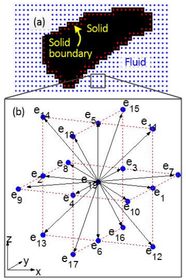
Dissipation consistency

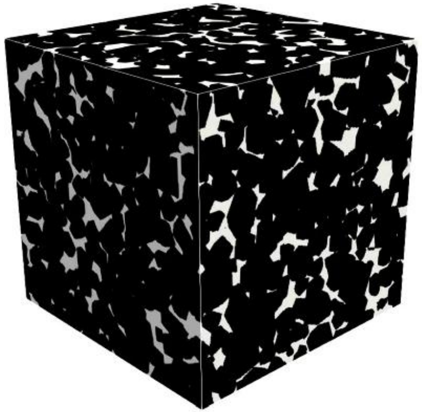
RVE must be statistically representative!

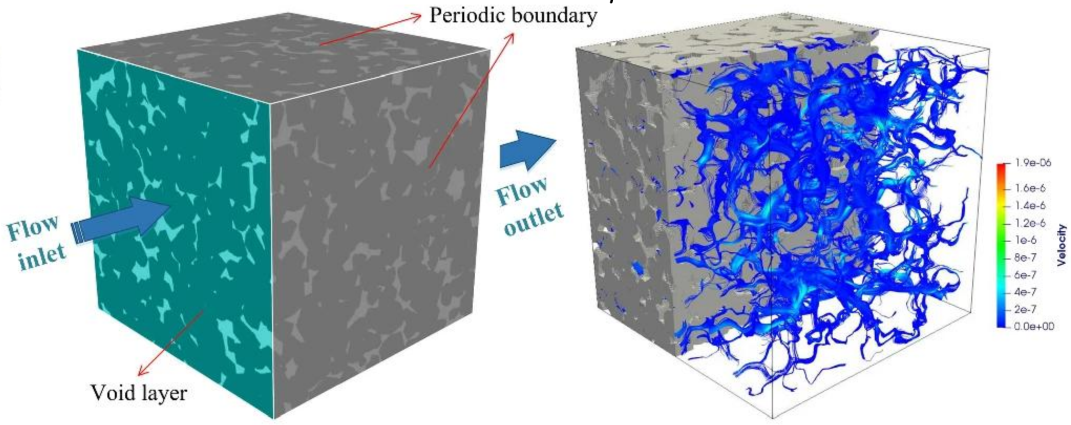
Macroscale:
Darcy flow. Impose pressure differential, measure velocities, and use them to get effective permeability

$$\frac{\partial}{\partial t}(\phi \rho^f) + \boldsymbol{\nabla}_{\boldsymbol{x}} \cdot (\rho^f \boldsymbol{q}^f) = Q^f$$

$$\boldsymbol{q}^f = -\frac{\boldsymbol{k}}{\mu}\nabla p \longrightarrow k_x = -\frac{\mu}{\nabla_x p}\langle q_x \rangle$$







Sun, Andrade and Rudnicki 2011 Int. J. Num. Meth. Eng.

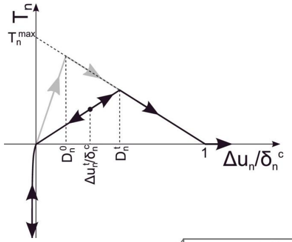
Fu et al 2020 Transp. Por. Med.

Homogenization for poromechanics

Rocks with cohesive interfaces

Microscale:
Grains separated by intefaces which open according to a cohesive law.

Macroscale:
Darcy flow with effective permeability upscaled from the microscale

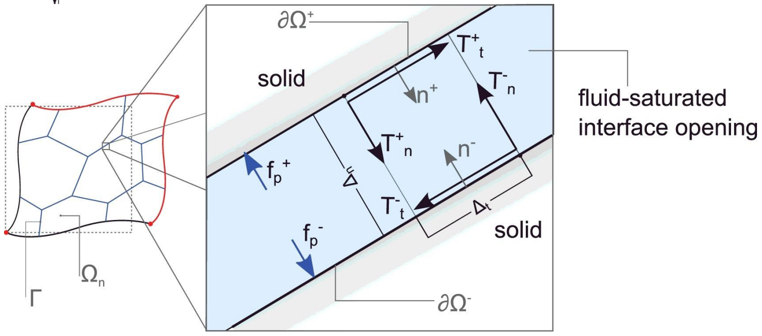


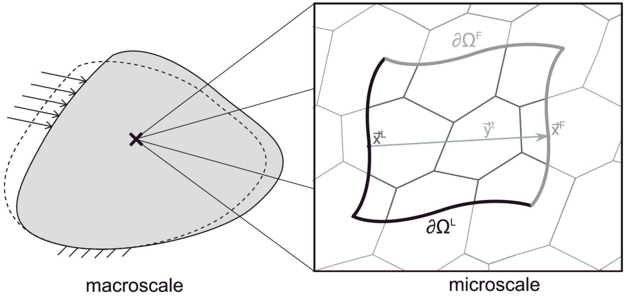
Assumption: Characteristic fluid timescale at microscale << macroscale
→ Steady-state laminar flow at microscale

$$\boldsymbol{\sigma}^M = \frac{1}{V}\int_{\partial V} \boldsymbol{t} \otimes \boldsymbol{x} dS$$

$$\nabla p^M = \frac{1}{V}\int_{\partial V} p^m \boldsymbol{n} dS$$

↑ Hydraulic pressure





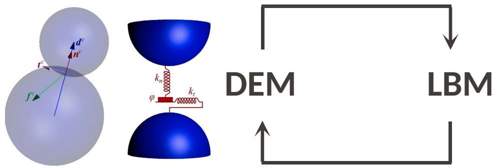
A.P. van den Eijnden et al 2016 Int. J. Sol. Struct.

Homogenization for poromechanics

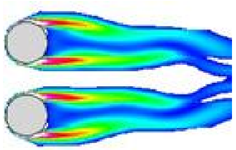
Saturated granular materials

The same methodology can be applied to granular assemblies by coupling DEM with a fluid solver e.g. **Lattice Boltzmann** (LBM).

Freeze particle positions



Freeze fluid velocities



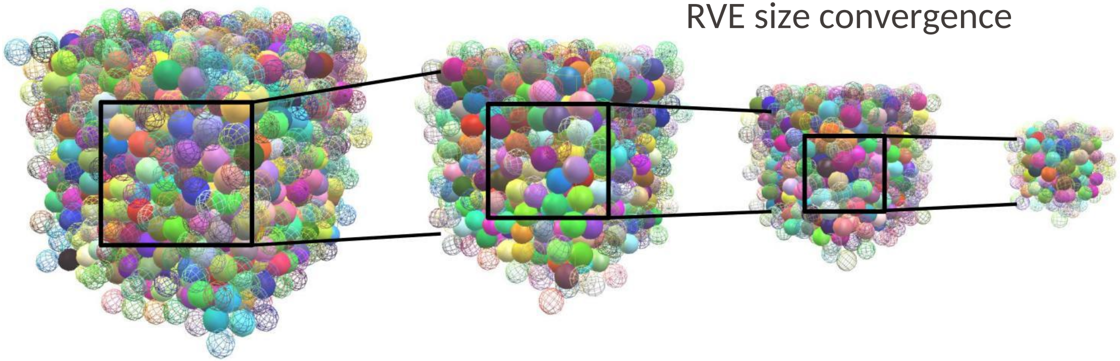
Macroscopic permeability:

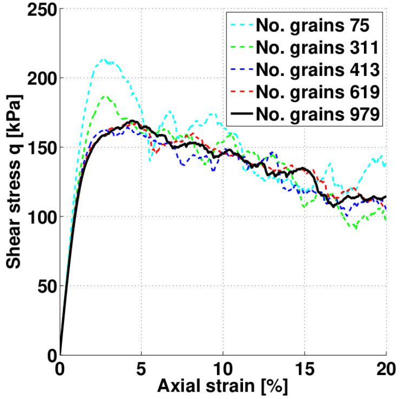
$$k_x = -\frac{\mu}{\nabla_x p}\langle q_x \rangle$$

$$\boldsymbol{\sigma} = \frac{1}{V}\sum_c \boldsymbol{l}^c \otimes \boldsymbol{f}^c - p^l \boldsymbol{I}$$

Can be extended to deformable skeleton!

RVE size convergence





Sun 2020 Alert Geomaterials

Homogenization for poromechanics

Unsaturated granular materials

The methodology can be extended to unsaturated granular materials via a multiphase fluid solver.

Fully saturated without flow

Pore space is filled with pressurized liquid.

$$\boldsymbol{\sigma} = \frac{1}{V}\sum_c \boldsymbol{l}^c \otimes \boldsymbol{f}^c - p^l \boldsymbol{I}$$

↑ Pore pressure

Unsaturated

Pore space is filled with liquid and gas, each with their own pressure.

Case of high saturation ratio:

$$\boldsymbol{\sigma} = \frac{1}{V}\sum_c \boldsymbol{l}^c \otimes \boldsymbol{f}^c - p^l \boldsymbol{I}$$

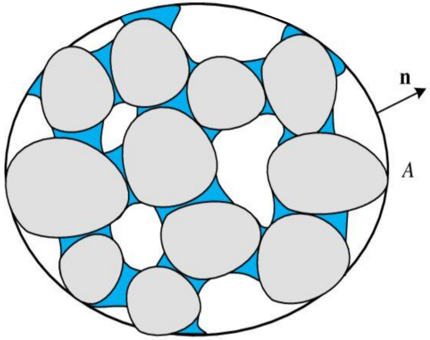
Case of low saturation ratio:

$$\boldsymbol{\sigma} = \frac{1}{V}\sum_c \boldsymbol{l}^c \otimes (\boldsymbol{f}^c + \boldsymbol{r}^c) - p^g \boldsymbol{I}$$

↑ Capillary force exerted by menisci

$$\boldsymbol{r}^c = \int_{\omega^{sl}} (p^g - p^l)\boldsymbol{n}dS + \int_{\partial\omega^{slg}} \gamma^{lg}\boldsymbol{v}ds$$

↑ Surface tension

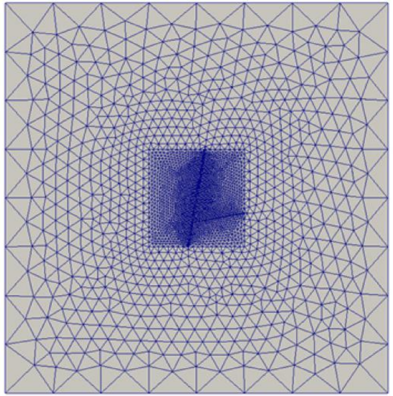


Chateau, Moucheront and Pitoiset 2002 J. Eng. Mech.

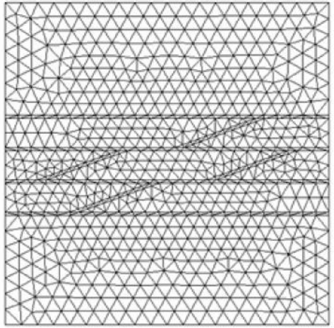
Homogenization for poromechanics

Data-driven approches

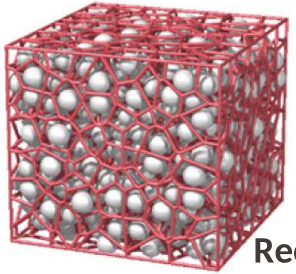
Macroscale
(FEM)



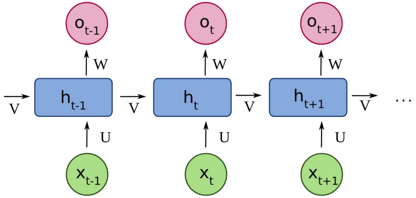
Mesoscale
(FEM)



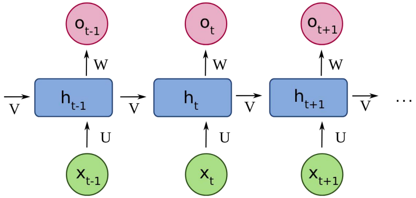
Microscale
(DEM, PNM)



Replaced by
Recurrent Neural Network (RNN)



Replaced by
RNN



Wang, and Sun 2018 Comp. Meth. Appl. Mech. Eng.

Homogenization in multiphysics problems

K. Karapiperis

- Poromechanics
- Heat conduction
- Thermoporomechanics
- Chemomechanics

Homogenization for heat conduction

Formulation - Asymptotic homogenization

This methodology assumes the presence of "**small parameters**" or separated scales in the system, s.t. the temperature field can be written as:

$$\theta(\boldsymbol{x}, \boldsymbol{y}) = \theta^0(\boldsymbol{x}, \boldsymbol{y}) + \epsilon\theta^1(\boldsymbol{x}, \boldsymbol{y}) + \epsilon^2\theta^2(\boldsymbol{x}, \boldsymbol{y}) + \dots$$

$$\boldsymbol{y} = \boldsymbol{x}/\epsilon$$

↑ Microscopic space variable

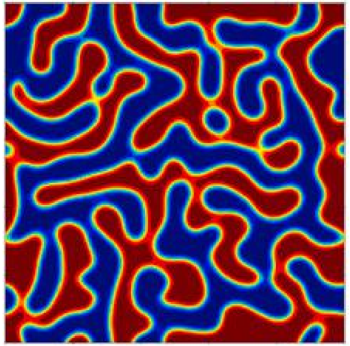
At each phase *i*, the heat conduction is governed by:

$$\nabla \cdot (k_i \nabla \theta_i) = \rho_i C_i \dot{\theta}_i$$

Let's consider a 2-phase system with strong contrasts:

$$k_1 = \mathcal{O}(1), k_2 = \mathcal{O}(\epsilon^2)$$

Inserting the temperature field, and using scaling arguments, allows us to obtain a homogenized equation, where effective conductivity only comes from phase 1, phase 2 (insulator) contributes to a memory term due to its thermal capacity and delayed release of heat.



You separate into a hierarchy of different problems!

J.L Auriault 1983 Int. J. Heat Mass Transfer

Homogenization for heat conduction

K.Karapiperis

Formulation - Computational homogenization

Microscale:
Time variation of heat storage is neglected due to the small RVE size, hence assume steady state conduction:

$$\nabla_m \cdot \boldsymbol{q}_m(\boldsymbol{x}) = 0 \qquad \boldsymbol{q}_m = -k_m \nabla_m \theta_m$$

Macro-to-micro transition:

$$\theta_m(\boldsymbol{x}) = \theta_M^0 + \nabla_M \theta_M (\boldsymbol{x} - \boldsymbol{x}^o) + \theta_f(\boldsymbol{x})$$

↑ Fluctuations

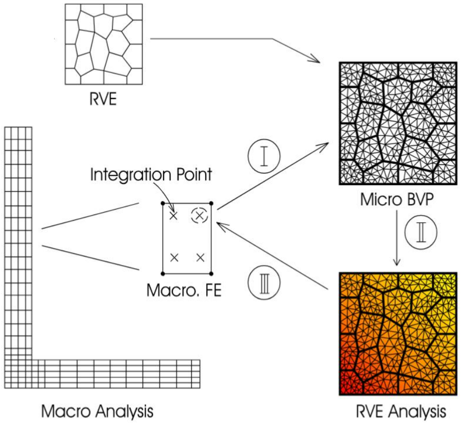
BCs satisfying:

$$\int_{\partial\Omega} \theta_f \boldsymbol{n} dS = \boldsymbol{0}$$

Macroscale:
The general time-dependent heat balance equation holds:

$$(\rho c_v)_M \dot{\theta}_M + \nabla_M \cdot \boldsymbol{q}_M = 0$$

↑ Macroscopic heat capacity



Ozdemir, Brekelmans and Geers 2008 Int. J. Num. Meth. Eng.

Volume averaging:

$$(\rho c_v)_M = \frac{1}{V} \int_V (\rho c_v)_m dV$$

$$\boldsymbol{q}_M = \frac{1}{V} \int_V \boldsymbol{q}_m dV$$

Effective conductivity obtained analytically or numerically (perturbations)

Homogenization for heat conduction

Applications in structural wood

Microscopic problem:

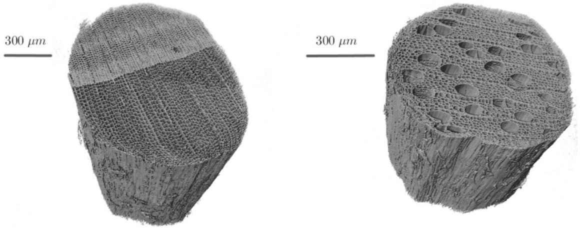
$$\nabla_m \cdot \boldsymbol{q}_m(\boldsymbol{x}) = 0$$

$$\boldsymbol{q}_m = -k_m \nabla_m \theta_m$$

↑

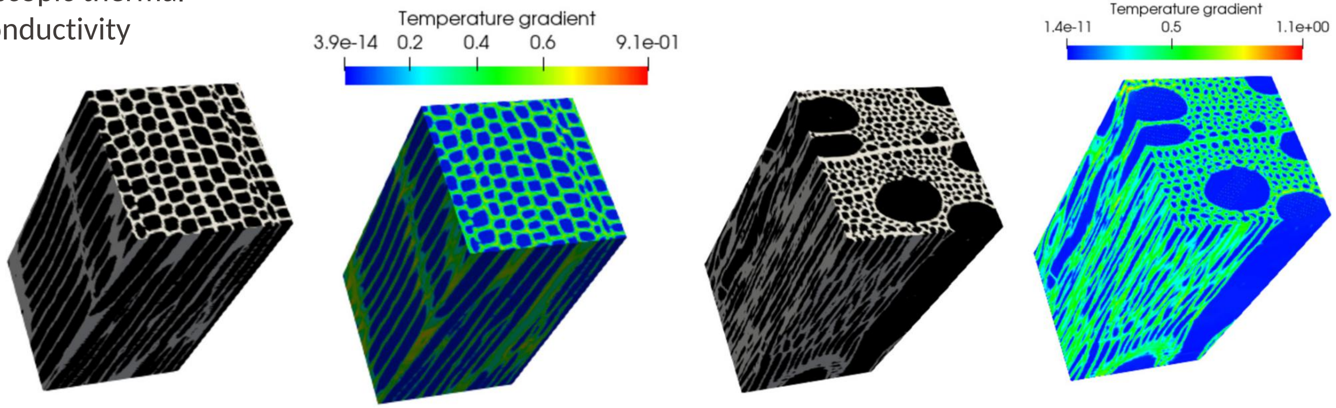
Microscopic thermal conductivity

Digital models of spruce and poplar wood



Homogenized conductivity:

$$k_x^M = \frac{q_x^{\partial \Omega^D} (x_r - x_l)}{\delta \theta_{rl}}$$



Mazian et al 2007 Int. J. Heat Mass Tran.

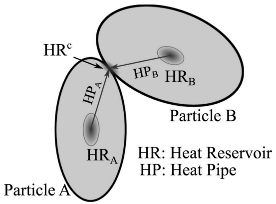
Homogenization for heat conduction

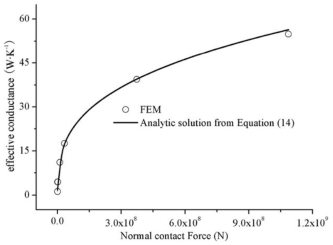
Applications to granular materials

Microscale:
Here we consider a discrete transient heat equation:

$$\rho_i c_i V_i \dot{\theta}_i = \sum_{j \in \mathcal{N}(i)} h_{ij}(\theta_i - \theta_j)$$

Heat conductivity (due to contact, etc) obtained e.g. from FEM simulations or adopting analytical solutions





Each particle has one temperature (instantaneous heat transfer within it)

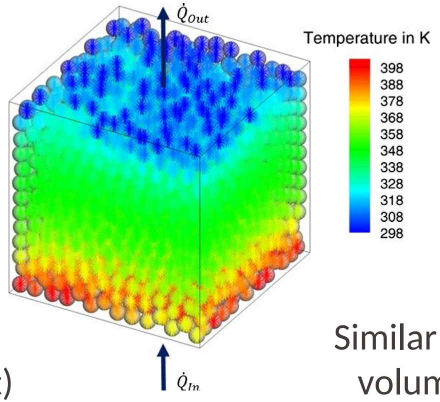
Macroscale:
The general time-dependent continuum heat equation holds:

$$(\rho c_v)_M \dot{\theta}_M + \nabla_M \cdot \boldsymbol{q}_M = 0 \quad \boldsymbol{q}_M = -\boldsymbol{k}_M \nabla \theta_M$$

Effective thermal conductivity

$$k_x^M = \frac{\langle q_x \rangle}{\langle \nabla_x \theta \rangle}$$

(Full tensor may be computed by solving RVE problem along many directions)



Similar can obtain effective heat capacity as volume average of particle heat capacities

Zhang et al 2011 Powder Technology

Homogenization for thermomechanics

Continuum to continuum

Microscale:
Time variation of heat storage is neglected due to the small RVE size, hence assume steady state heat conduction:

$$\nabla_m \cdot \boldsymbol{q}_m(\boldsymbol{x}) = 0$$

$$\nabla_m \cdot \boldsymbol{\sigma}_m(\boldsymbol{x}) = 0$$

Micro-Macro consistency

$$\boldsymbol{P}_M : \dot{\boldsymbol{F}}_M = \frac{1}{V_0}\int_{V_0} \boldsymbol{P}_m : \dot{\boldsymbol{F}}_m dV_0$$

$$\nabla_M \theta_M \cdot \boldsymbol{q}_M = \frac{1}{V}\int_V \nabla_m \theta_m \cdot \boldsymbol{q}_m dV$$

Macroscale:
The general time-dependent heat balance and momentum balance equations hold:

$$(\rho c_v)_M \dot{\theta}_M + \nabla_M \cdot \boldsymbol{q}_M = 0$$

$$\nabla_M \cdot \boldsymbol{\sigma}_M = 0$$

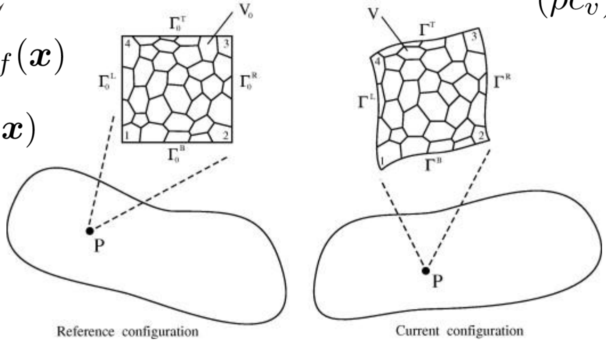
Macro-to-micro transition:

Fluctuations ↓

$$\theta_m(\boldsymbol{x}) = \theta_M^0 + \nabla_M \theta_M(\boldsymbol{x} - \boldsymbol{x}^o) + \theta_f(\boldsymbol{x})$$

$$\boldsymbol{u}_m(\boldsymbol{x}) = (\boldsymbol{F}_M - \boldsymbol{I})(\boldsymbol{X} - \boldsymbol{X}^o) + \boldsymbol{u}_f(\boldsymbol{x})$$

Enforce $\boldsymbol{F}_M, \nabla_M \theta_M$ through periodic BCs



Ozdemir, Brekelmans and Geers 2008 Comp. Meth. Appl. Mech. Eng.

Volume averaging:

$$(\rho c_v)_M = \frac{1}{V}\int_V (\rho c_v)_m dV$$

$$\boldsymbol{q}_M = \frac{1}{V}\int_V \boldsymbol{q}_m dV$$

$$\boldsymbol{P}_M = \frac{1}{V_0}\int_{V_0} \boldsymbol{P}_m dV_0$$

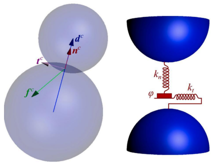
Effective conductivity and stiffness obtained analytical or numerically

Homogenization for thermomechanics

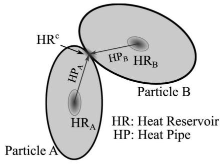
Discrete to continuum

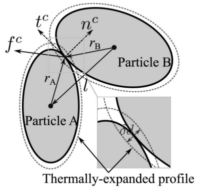
Microscale:
Transient heat conduction through a heat-pipe model (HPM) and standard DEM modeling.

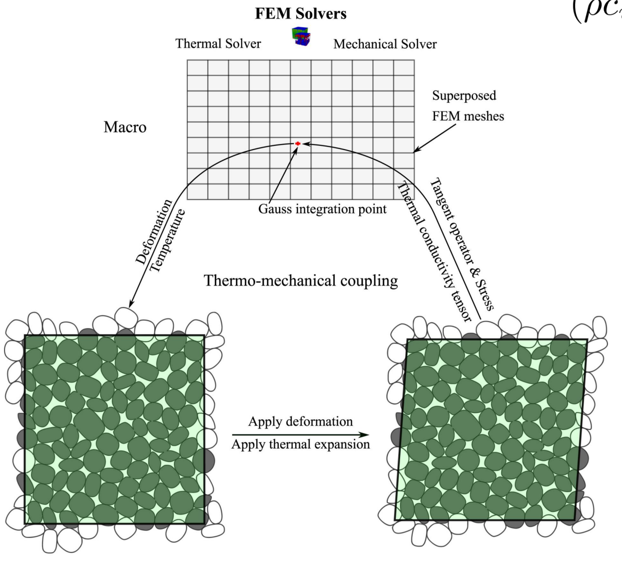
$$\rho_i c_i V_i \dot{\theta}_i = \sum_{j \in \mathcal{N}(i)} h_{ij}(\theta_i - \theta_j)$$



Freeze particle positions → DEM
HPM ← Freeze particle temperatures







Zhao, Zhao and Lai 2020 Comp. Meth. Appl. Mech. Eng.

Macroscale:
The general time-dependent heat balance and momentum balance equations hold:

$$(\rho c_v)_M \dot{\theta}_M + \nabla_M \cdot \boldsymbol{q}_M = 0$$

$$\nabla_M \cdot \boldsymbol{\sigma}_M = 0$$

Effective properties:

Therm.:

$$\boldsymbol{q}_M = \frac{1}{V} \sum_p \boldsymbol{q}^p A^p l^p$$

$$\boldsymbol{k} = \frac{1}{V} \sum_p \frac{\boldsymbol{r}^p \otimes \boldsymbol{r}^p}{a^p l^p}$$

← Heat pipe parameters

Mech.:

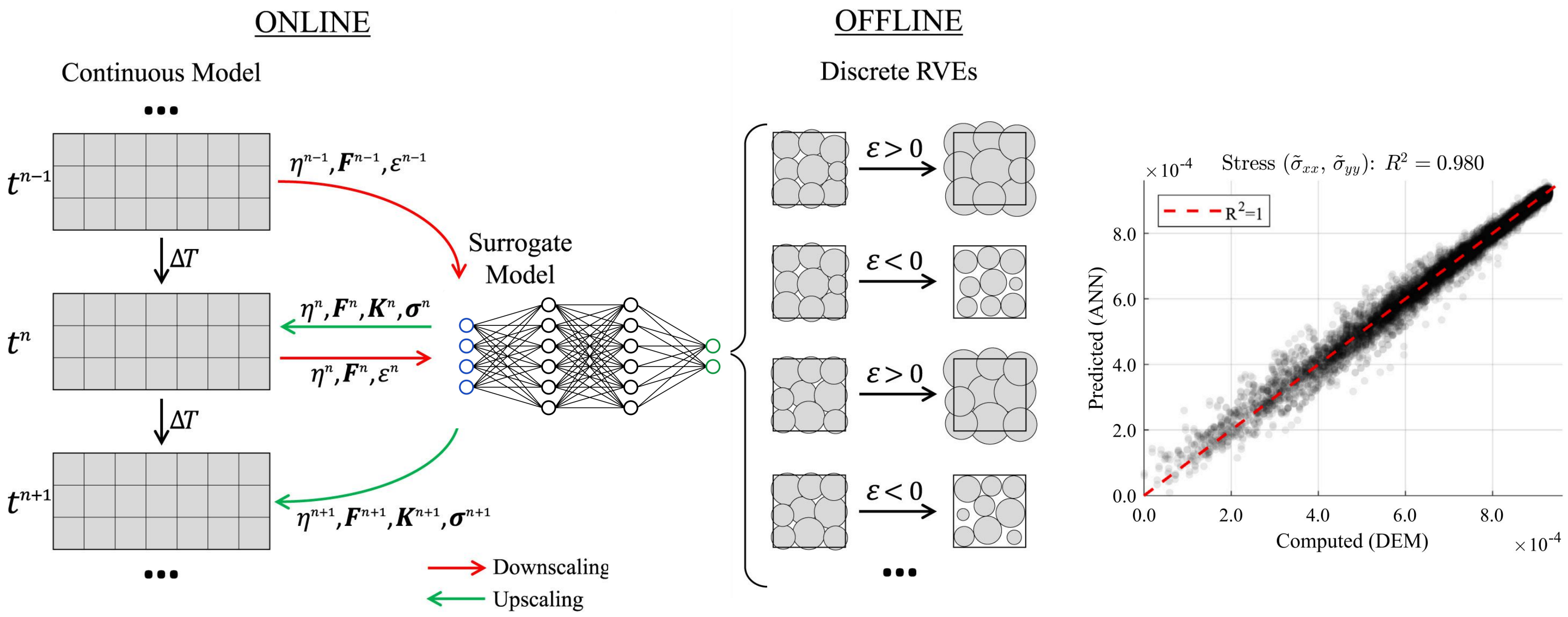
$$\boldsymbol{\sigma}_M = \frac{1}{V} \sum_c \boldsymbol{l}^c \otimes \boldsymbol{f}^c$$

$$\boldsymbol{C} = \frac{1}{V} \sum_c k_n \boldsymbol{n}^c \otimes \boldsymbol{l}^c \otimes \boldsymbol{n}^c \otimes \boldsymbol{l}^c + \frac{1}{V} \sum_c k_t \boldsymbol{t}^c \otimes \boldsymbol{l}^c \otimes \boldsymbol{t}^c \otimes \boldsymbol{l}^c$$

Homogenization for thermomechanics

Data-driven approches

Machine learning and model-free data-driven approaches may be used to accelerate thermomechanical (and similarly other coupled) multiscale calculations. The same DEM and heat-pipe model can be used to create a dataset corresponding to different porosities



Rangel et al 2024 Comp. Geotech.

Homogenization for thermoporomechanics

Discrete to continuum

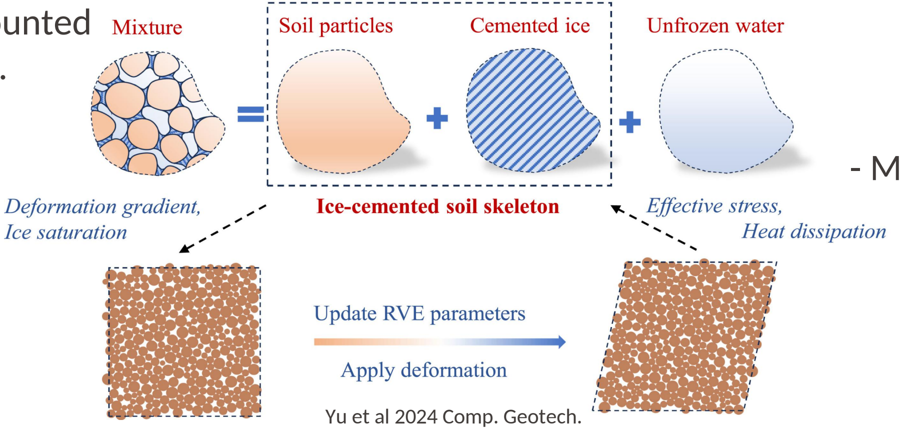
The techniques presented for the poromechanical and the thermomechanical problem are readily extendable to a fully coupled thermohydromechanical problem, e.g.:

Microscale:
In principle can consider all effects at the microscale (mechanical interactions, flow, phase change to ice). Here only the mechanical interactions are accounted for at the microscale.

Macroscale:
A three-phase continuum described by solid volume fraction and ice percentage. Assumes Darcy-type fluid flow, Fourier-type heat conduction.

↓

- Mass balance
- Momentum Balance
- Energy balance



Yu et al 2024 Comp. Geotech.

Homogenization in multiphysics problems

- Poromechanics
- Heat conduction
- Thermoporomechanics
- Chemomechanics

Homogenization in chemomechanics

Concrete corrosion

Microscale:
Momentum balance, ion diffusion and phase-field fracture.

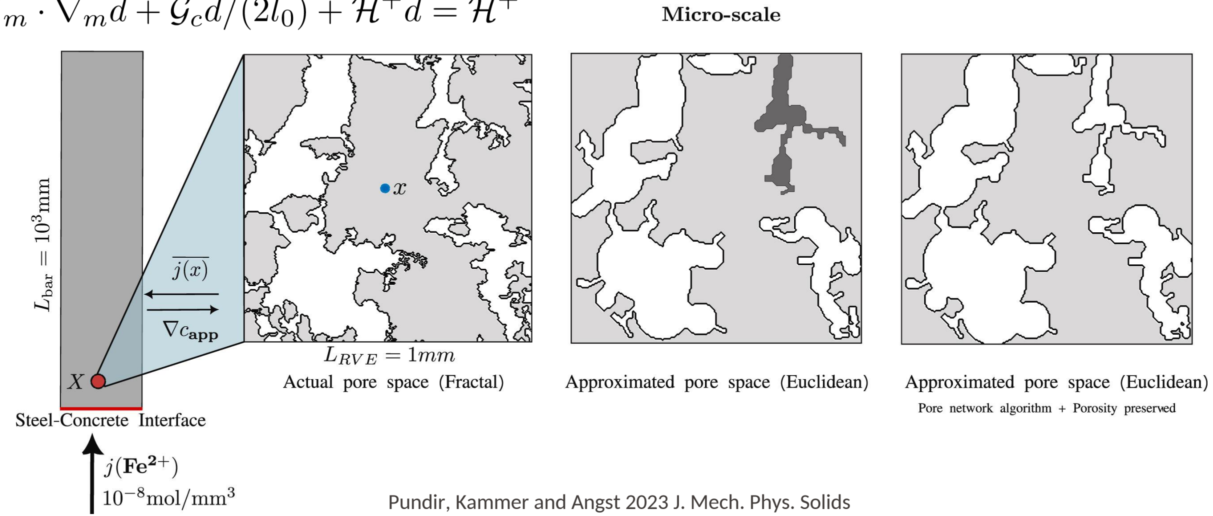
$$\nabla_m \cdot \boldsymbol{\sigma}_m(\boldsymbol{x}) = 0$$
$$\nabla_m \cdot \boldsymbol{j}_m(\boldsymbol{x}) = 0$$
$$-1/2\mathcal{G}_c l_0 \nabla_m \cdot \nabla_m d + \mathcal{G}_c d/(2l_0) + \mathcal{H}^+ d = \mathcal{H}^+$$

Equations solved in Fourier space using FFT.

Macroscale:
Momentum balance and ion diffusion.

$$\nabla_M \cdot \boldsymbol{\sigma}_M = 0$$
$$\nabla \cdot \boldsymbol{j}_M = 0$$

Macroscopic damage due to microcracking

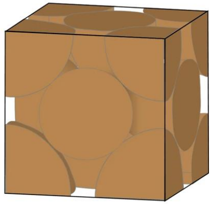


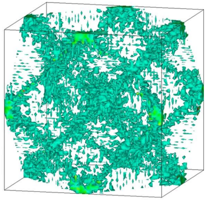
Pundir, Kammer and Angst 2023 J. Mech. Phys. Solids

Homogenization in chemomechanics

Biocemented geomaterials

Microscale:
Momentum balance, reaction diffusion





RVE

Macroscale:
Same physics.
Stress and stiffness extracted from the microscale

$$\frac{\partial A}{\partial t} = \nabla\left(D_A \nabla A\right) - k_1 A B^2 + k_2 C E^2 + A_{\text{in}}$$

$$\frac{\partial B}{\partial t} = \nabla\left(D_B \nabla B\right) - k_1 A B^2 + 2k_2 C E^2 + B_{\text{in}}$$

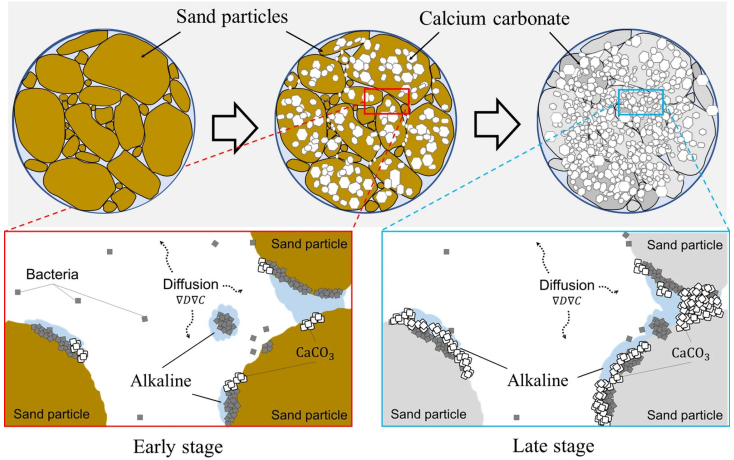
$$\frac{\partial C}{\partial t} = \nabla\left(D_C \nabla C\right) + k_1 A B^2 - k_2 C E^2 - k_3 C F + k_4 P$$

$$\frac{\partial E}{\partial t} = \nabla\left(D_E \nabla E\right) + 2k_1 A B^2 - k_2 C E^2$$

$$\frac{\partial F_{\text{i}}}{\partial t} = \frac{\partial}{\partial x} D_{\text{F}} \frac{\partial F_{\text{i}}}{\partial x} - k_3 C_{\text{i}} F_{\text{i}} + k_4 P + F_{\text{in}}$$

$$\frac{\partial P}{\partial t} = k_3 C_{\text{i}} F_{\text{i}} - k_4 P$$

Calcium carbonate concentration



Nishimura and Matsubara 2021 Acta Geotechnica

Extension to other multiphysics problems

A variety of many other interesting multiphysics problems may be tackled with similar techniques including:

- Electromechanics (smart structures, active dampers, etc)
- Magnetomechanics (shape memory alloys, magneto-rheological dampers)
- Thermoelectromechanics (batteries)
- Chemomechanics (corrosion, hydrogen embrittlement)
- Thermochemomechanics (concrete hydration, polymer curing)
- Optomechanics (photoelasticity where stress causes birefringence)
- Radiation (nuclear geobarriers and structural vessel)

Discussion

That's what I prepared for you today.

What would you like to discuss?

Outlook

Final presentations

(See Moodle announcement for details)