Mini-workshop on

Jamming, rheology and granular matter

Kyoto, Japan – July 9, 2025

YUKAWA INSTITUTE FOR THEORETICAL PHYSICS

A Data-Driven Framework for Efficient Hierarchical Multiscale Modeling of Thermomechanical Effects in Granular Materials

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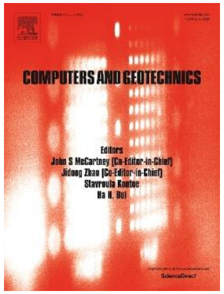
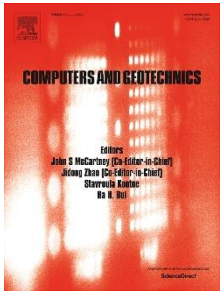
CIMNE International Centre for Numerical Methods in Engineering

Reference Publications

R.L. Rangel, J.M. Gimenez, E. Oñate, and A. Franci.
A continuum–discrete multiscale methodology using machine learning for thermal analysis of granular media.
Computers and Geotechnics, 168:106118, 2024.



R.L. Rangel, A. Franci, E. Oñate, and J.M. Gimenez.
Multiscale data-driven modeling of the thermomechanical behavior of granular media with thermal expansion effects.
Computers and Geotechnics, 176:106789, 2024.



1 – Introduction

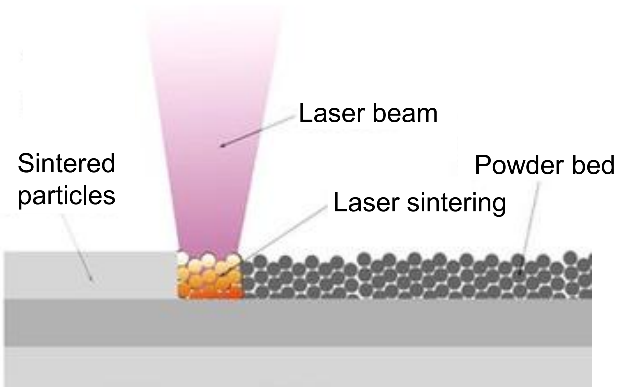
2 – Methodology

3 – Results and Discussions

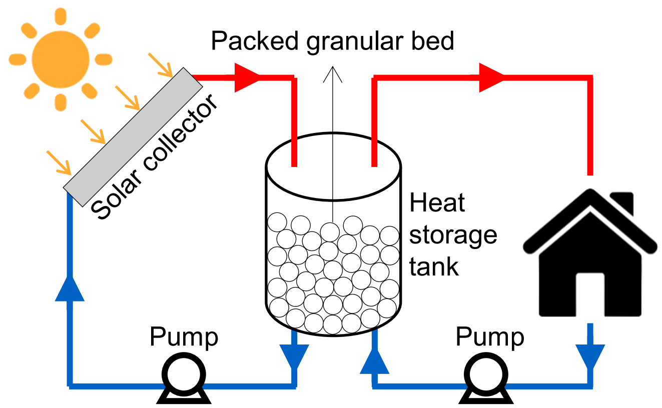
4 – Conclusions

Motivation

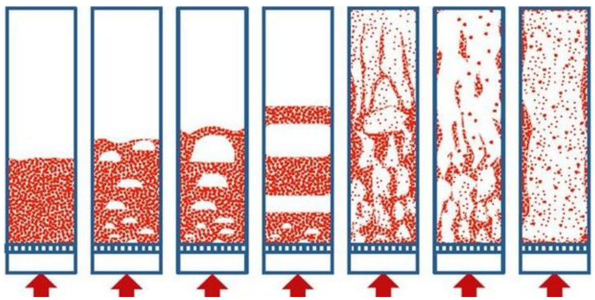
Thermomechanical effects in granular materials



Selective laser sintering

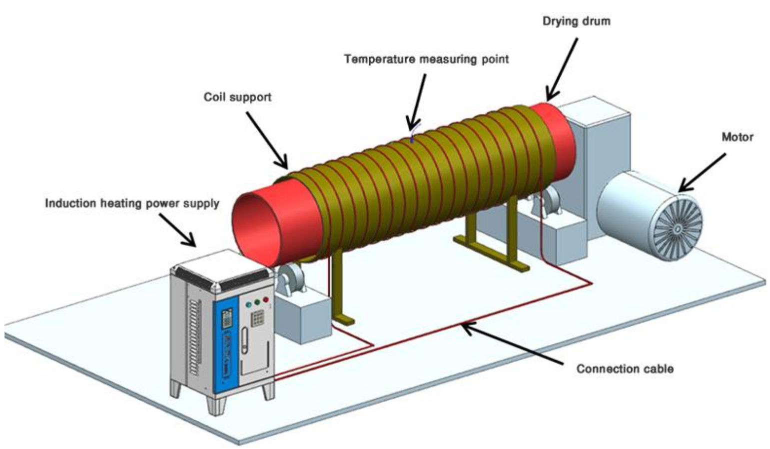


Thermal energy storage systems



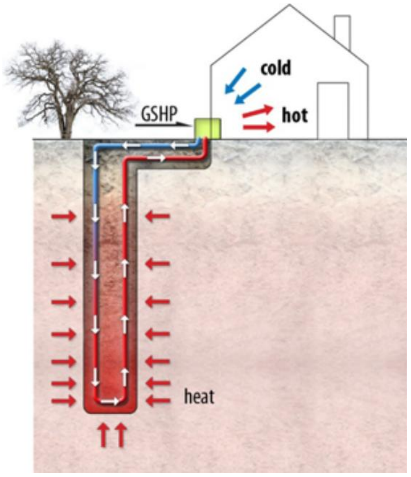
Fluidized beds in catalytic reactors

Adham and Bowes, 1st Global Conference on Extractive Metallurgy, 2505-2512, 2018



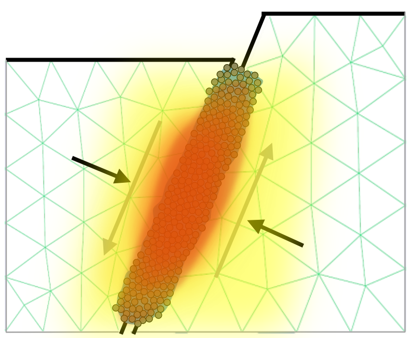
Rotating drum driers

http://inductionheater-inc.com/induction-heating-for-rotary-drum-dryer.html



Geothermal piles

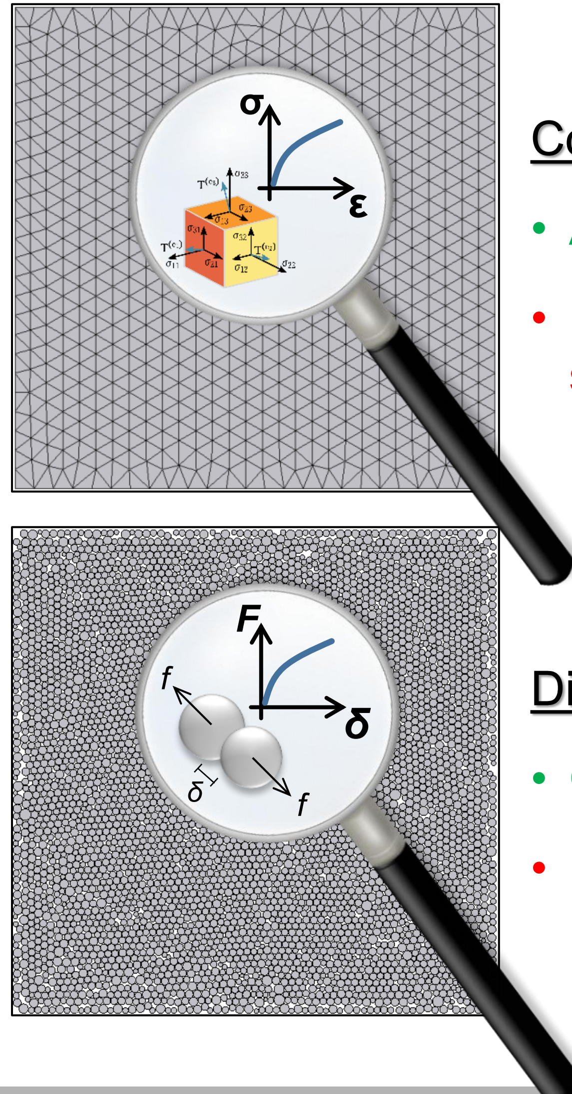
Johnston, *KSCE J. Civil Eng.*,15:643-653, 2011



Flash frictional heating in seismic activities

Modeling Limitations

Dichotomy of numerical approaches for granular media



<u>Continuous methods</u>

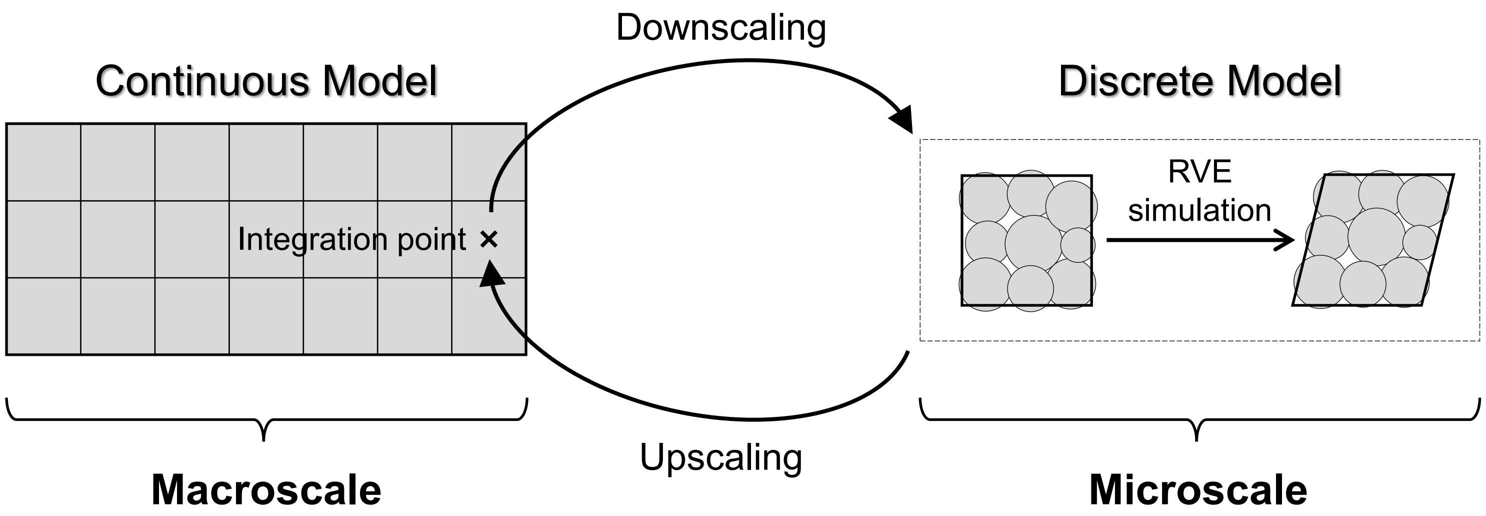
- Affordable computational cost.
- Phenomenological, scale-specific constitutive laws.

<u>Discrete methods (DEM)</u>

- Grain-scale accuracy.
- High computational cost.

Modeling Limitations

Continuum-discrete hierarchical multiscale



- Alleviates the limitations of continuous and discrete methods.
- Online (runtime) RVE simulations: Too expensive for real-world problems.
- Seldom applied to investigate thermomechanical effects.

Objectives

Multi-Scale Data-Driven (MSDD) approach

High-fidelity simulations

Accuracy from the discrete method

Fast simulations

Efficiency from the continuous method

Ingredients

Continuum-discrete hierarchical multiscale

Pre-computed microscale solutions

Machine-learning surrogate model

Purpose: Thermomechanical analyses

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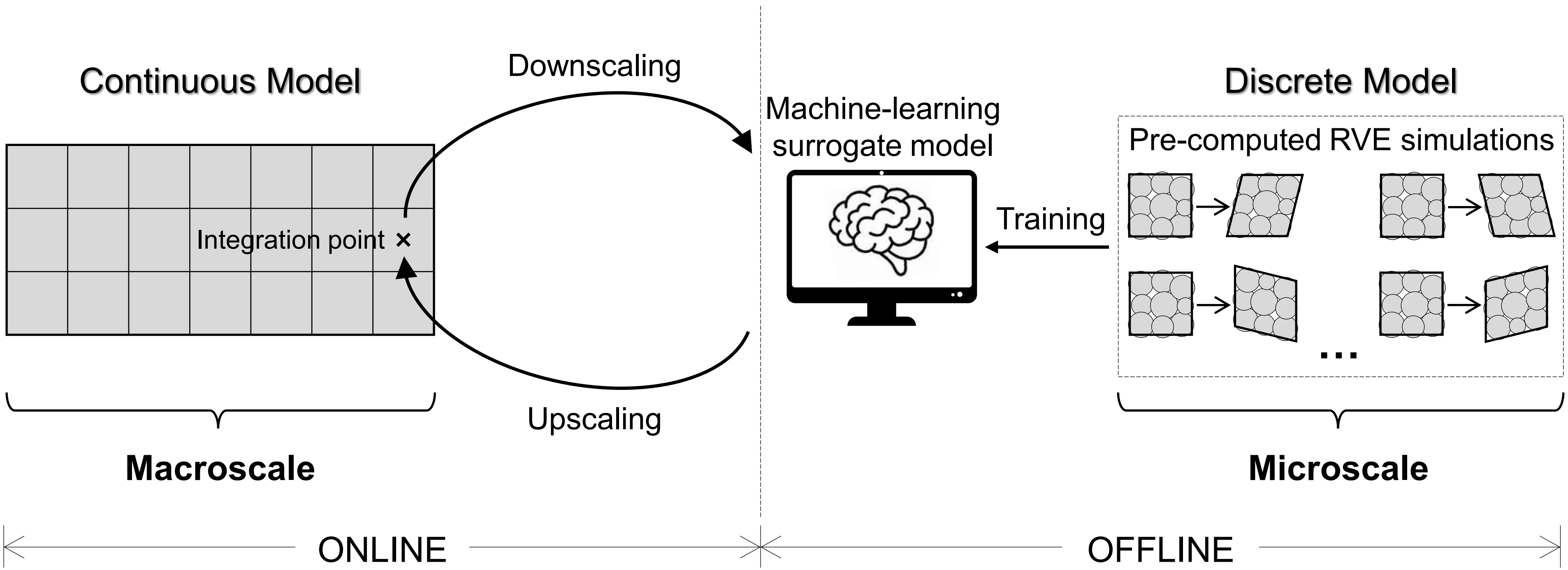
General Scheme

Multi-Scale Data-Driven (MSDD) approach



Current scope:
- Thermal effects: heat conduction + thermal expansion
- Small deformations in confined systems
- Two-dimensional (2D) models with no gravity

Specific Scheme

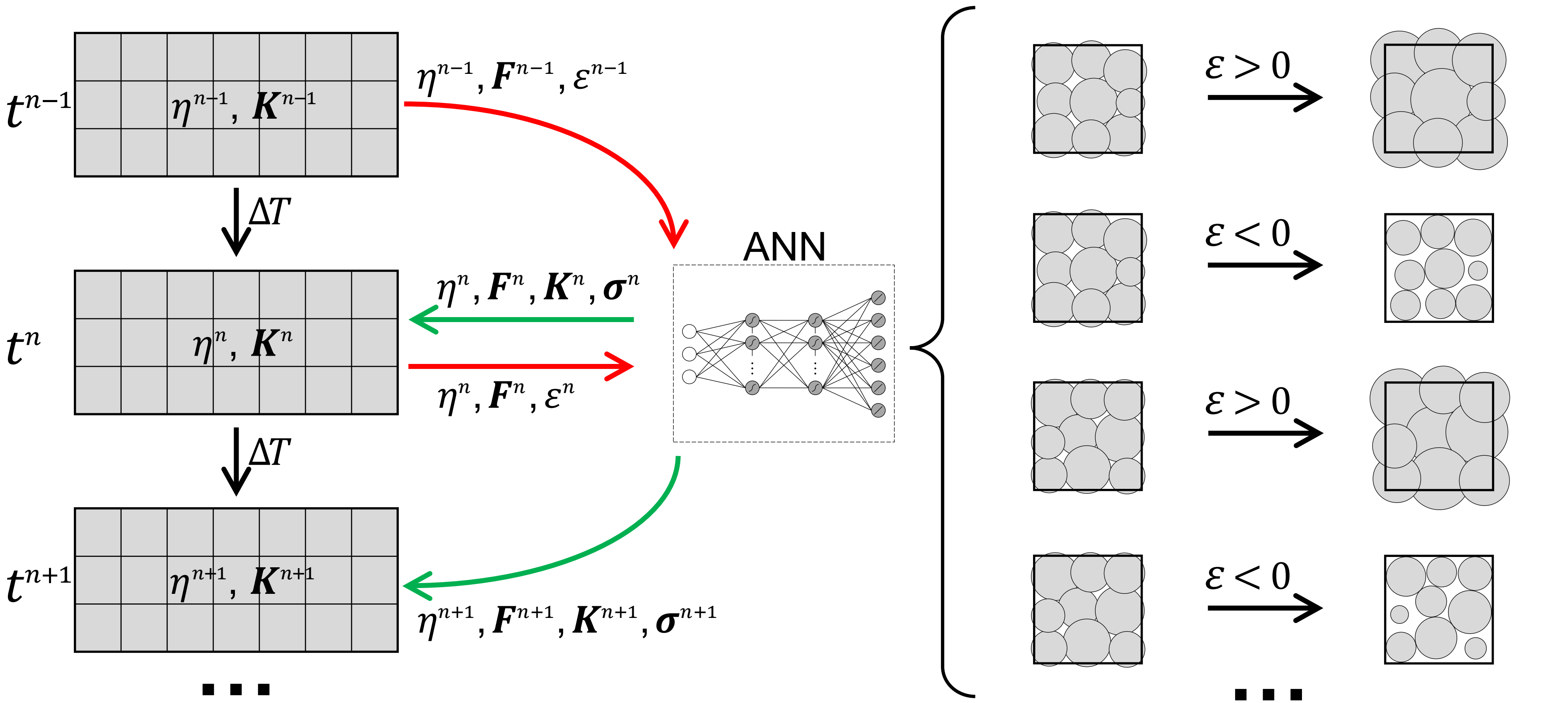
Continuous model

$$\rho_s(1-\eta)\frac{\partial T}{\partial t} = \nabla \cdot (\boldsymbol{K}\nabla T)$$

DEM RVEs

Input config. $(\eta, \boldsymbol{F})_0$

Output config. $(\eta, \boldsymbol{F}, \boldsymbol{K}, \boldsymbol{\sigma})_{\mathrm{i}}$



T: Temperature ρ_s: Solid density η: Porosity $\boldsymbol{F}$: Fabric ε: Thermal strain $\boldsymbol{K}$: Conductivity $\boldsymbol{\sigma}$: Stress

Macroscale Continuum Solver

Transient heat diffusion problem

$$\varrho c \frac{\partial T}{\partial t} = \nabla \cdot (\boldsymbol{K} \nabla T) \quad \text{in } [\Omega, t] \quad \text{where: } \varrho = \rho_s(1-\eta)$$

$$T = \overline{T} \quad \text{in } [\Gamma_{\mathrm{D}}, t]$$

$$\boldsymbol{K} \nabla T \cdot \boldsymbol{n}_\Gamma = \overline{q} \quad \text{in } [\Gamma_{\mathrm{N}}, t]$$

$$T = T_0 \quad \text{in } [\Omega, 0]$$

OpenFOAM

Finite Volume Method (FVM)

$$\sum_i \left((\varrho c)_i \left(\frac{\partial T}{\partial t} \right)_i \Omega_i - \sum_{b \in \Gamma_i} (\boldsymbol{K} \cdot \nabla T \cdot \boldsymbol{n})_b \, \Gamma_b \right) = 0$$

- Time integration scheme: Implicit 1st-order
- Spatial approximation: 2nd-order operators

Effective granular properties ($\boldsymbol{K}$, ϱc) depend on the current microstructure

Microscale Discrete (DEM) Solver

Equations of motion

$$\begin{cases} \dfrac{d\boldsymbol{v}}{dt} = \dfrac{\boldsymbol{f}}{m}, & \boldsymbol{f} = \boldsymbol{f}_d + \sum^{N_n} \boldsymbol{f}_n + \boldsymbol{f}_t \\ \dfrac{d\boldsymbol{\omega}}{dt} = \boldsymbol{I}^{-1}\boldsymbol{M}, & \boldsymbol{M} = \sum^{N_n} \boldsymbol{M}_{f_t} \end{cases}$$

Thermal energy

$$\left\{ \dfrac{dT}{dt} = \dfrac{q}{mc}, \quad q = \sum^{N_n} q_c \right.$$

Microscale Discrete (DEM) Solver

Equations of motion
$$\begin{cases} \dfrac{d\boldsymbol{v}}{dt} = \dfrac{\boldsymbol{f}}{m}, & \boldsymbol{f} = \boldsymbol{f}_d + \sum^{N_n} \boldsymbol{f}_n + \boldsymbol{f}_t \\ \dfrac{d\boldsymbol{\omega}}{dt} = \boldsymbol{I}^{-1}\boldsymbol{M}, & \boldsymbol{M} = \sum^{N_n} \boldsymbol{M}_{f_t} \end{cases}$$

Thermal energy
$$\begin{cases} \dfrac{dT}{dt} = \dfrac{q}{mc}, & q = \sum^{N_n} q_c \end{cases}$$

Mechanical interaction models (Linear forces + Coulomb friction + damping)

$\boldsymbol{f}_n = -s_n \delta_n \boldsymbol{n}$ where: $s_n = 2 e r_1 r_2 / (r_1 + r_2)$

$$\boldsymbol{f}_t = \begin{cases} \boldsymbol{f}_t^{\text{prev}} - \nu s_n \Delta \boldsymbol{u}_t & \text{if } \|\boldsymbol{f}_t\| \leq \|\boldsymbol{f}_n\| \tan(\varphi) \\ \|\boldsymbol{f}_n\| \tan(\varphi)\, \boldsymbol{t} & \text{otherwise} \end{cases}$$

$$\boldsymbol{f}_d = -\mu \|\boldsymbol{f}_c\| \frac{\boldsymbol{v}}{\|\boldsymbol{v}\|}$$

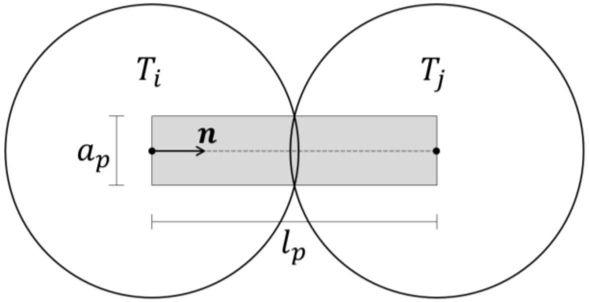
Microscale Discrete (DEM) Solver

Equations of motion
$$\begin{cases} \frac{d\boldsymbol{v}}{dt} = \frac{\boldsymbol{f}}{m}, & \boldsymbol{f} = \boldsymbol{f}_d + \sum^{N_n} \boldsymbol{f}_n + \boldsymbol{f}_t \\ \frac{d\boldsymbol{\omega}}{dt} = \boldsymbol{I}^{-1}\boldsymbol{M}, & \boldsymbol{M} = \sum^{N_n} \boldsymbol{M}_{f_t} \end{cases}$$

Thermal energy
$$\left\{ \frac{dT}{dt} = \frac{q}{mc}, \qquad q = \sum^{N_n} q_c \right.$$

Thermal interaction model (Thermal pipe model)

$$q_c = -k a_p \frac{(T_i - T_j)}{l_p}$$



Thermal expansion model (Linear model)

$\Delta r = \varepsilon r^0$ where, thermal strain: $\varepsilon = \alpha \Delta T$

Micro-to-Macro Upscaling Formulation

Fabric tensor

$$\boldsymbol{F} = \frac{1}{N_c}\sum_{N_c} \boldsymbol{n} \otimes \boldsymbol{n}$$

2D: $$\boldsymbol{F} = \begin{bmatrix} F_{xx} & F_{xy} \\ F_{xy} & F_{yy} \end{bmatrix}$$

Since $\mathrm{tr}(\boldsymbol{F}) = 1$ and $F_{xy} \cong 0$, $\boldsymbol{F}$ is represented as a scalar fabric index: $f = F_{xx} - F_{yy}$

Effective thermal conductivity tensor

$$\boldsymbol{K} = \frac{1}{V}\sum_{N_c} k a_p l_p \, \boldsymbol{n} \otimes \boldsymbol{n}$$

- Derived for thermal pipe model
- Geometry-based (no heat applied)
- k: Particles conductivity

Cauchy stress tensor

$$\boldsymbol{\sigma} = \frac{1}{V}\sum_{N_c} (-l_p \, \boldsymbol{n}) \otimes (\boldsymbol{f}_n + \boldsymbol{f}_t)$$

Mean effective stress: $$p = \frac{1}{dim}\mathrm{tr}(\boldsymbol{\sigma})$$

RVE Packing Generation

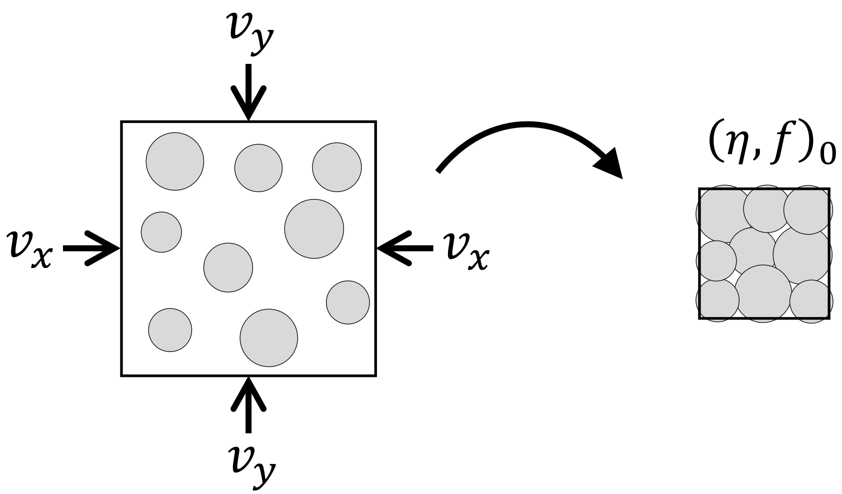
Particles randomly positioned
in a control volume

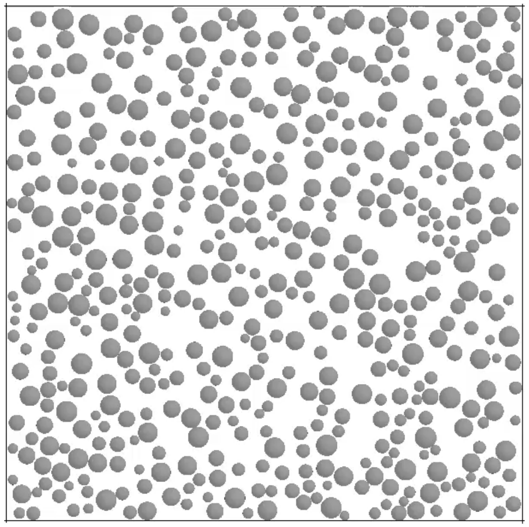
Compression by flat walls

No gravity

Compression stop criterion:
target packed porosity (η_0)

Relative wall velocities in X,Y directions
to modify packed fabric ($\boldsymbol{F}_0$)





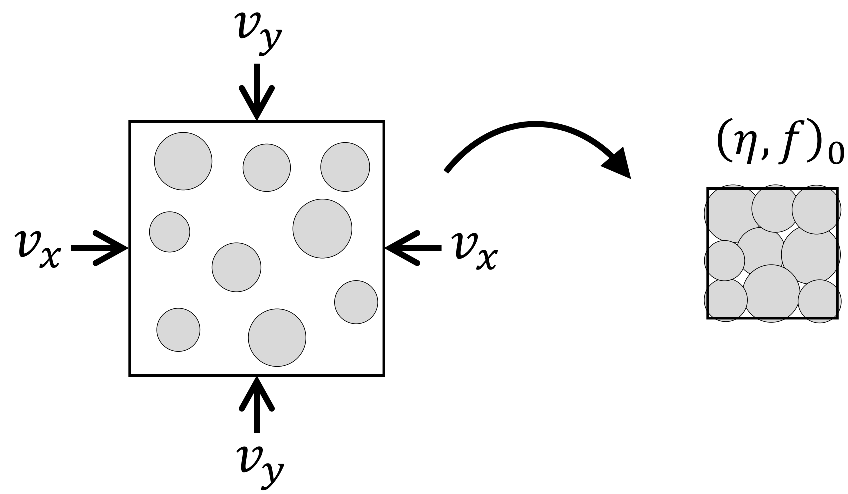
Particles <u>randomly positioned</u> in a control volume

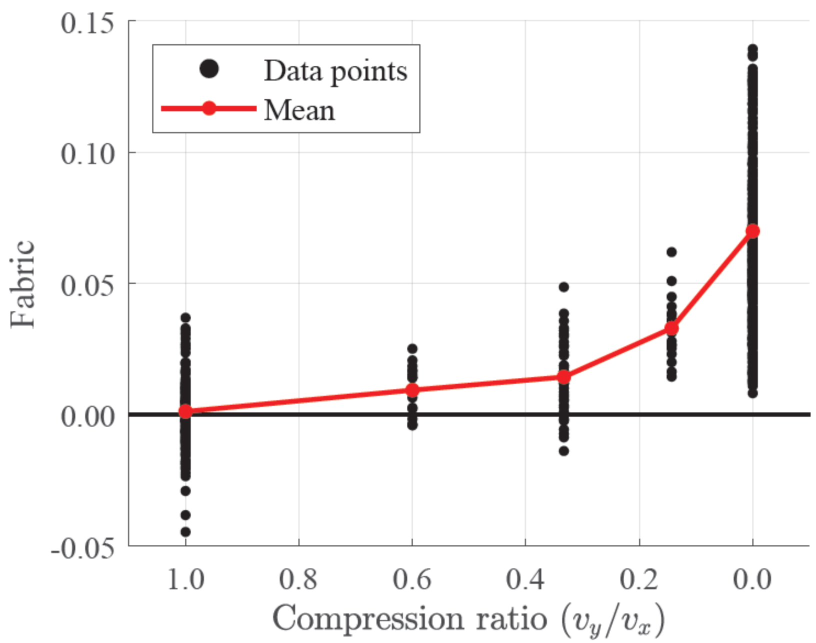
Compression by <u>flat walls</u>

<u>No gravity</u>

Compression <u>stop criterion</u>: target packed porosity (η_0)

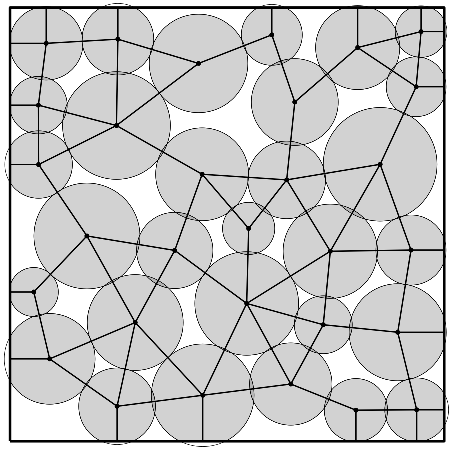
Relative wall velocities in X,Y directions to <u>modify packed fabric</u> ($\boldsymbol{F}_0$)

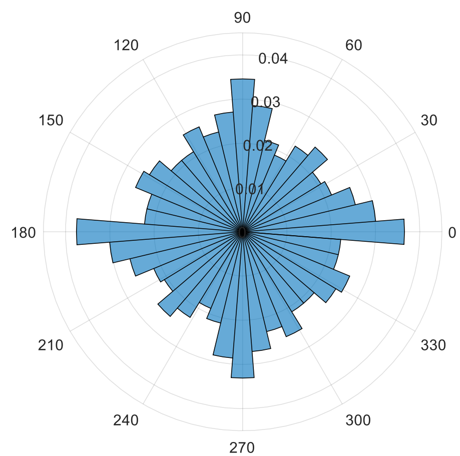




RVE Boundary Treatment

All contacts

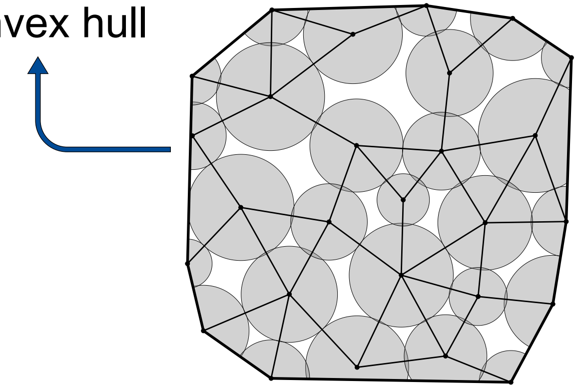


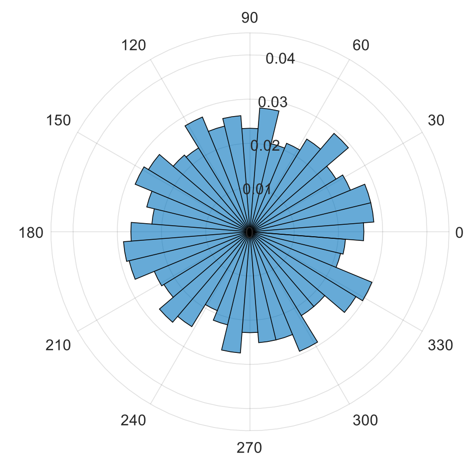


Predominance of main XY directions

Internal contacts

Convex hull

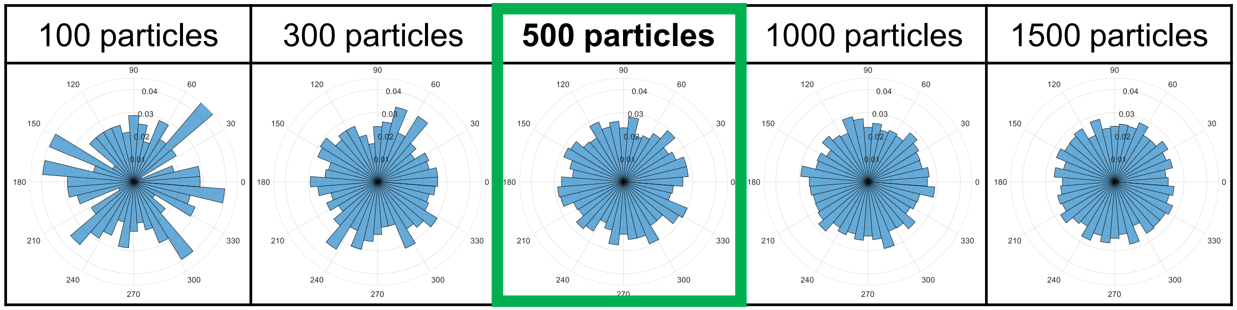




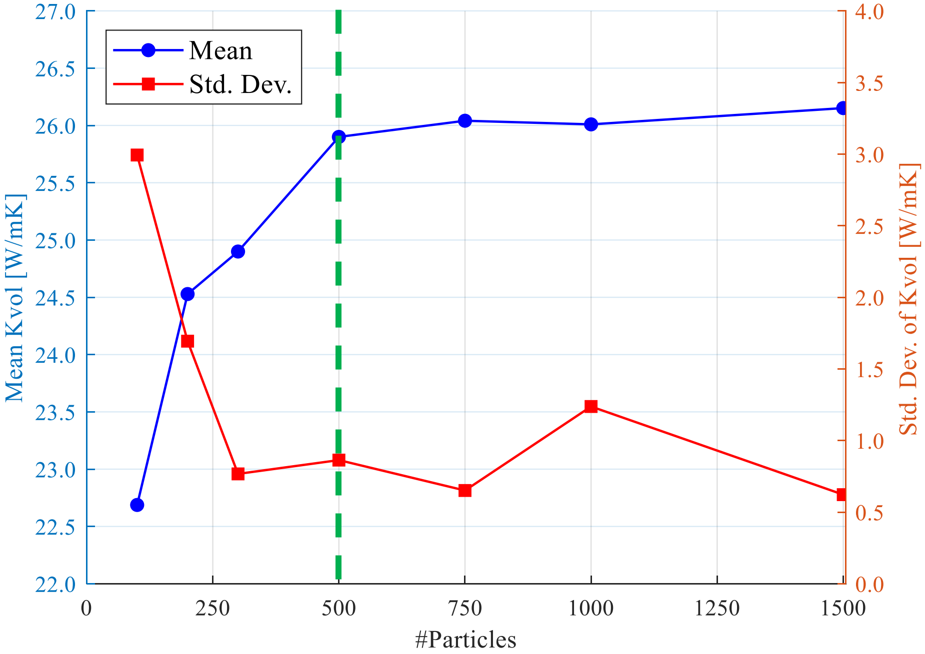
Wall effects are vanished

RVE Representativeness

Convergence of rose diagram



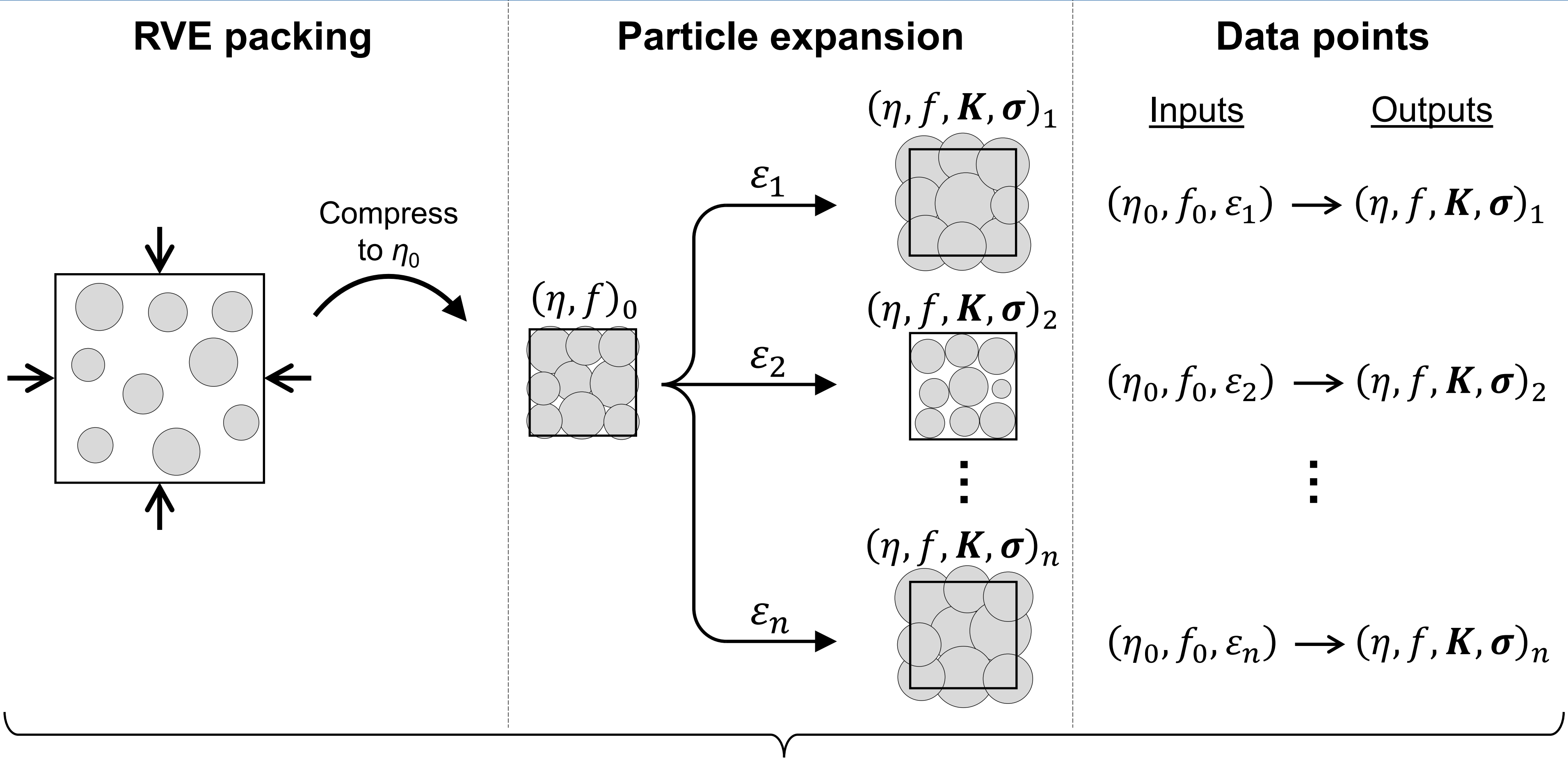
Convergence of effective conductivity



10 RVEs packings with different #particles

500 particles: Good balance between Computational Cost vs. Representativeness

Microscale Database Generation



Repeat for several packings $(\eta, f)_0$

Frame invariance:

- Simulated data points: $(\eta_0, f_0, \varepsilon) \rightarrow (\eta, f, \boldsymbol{K}, \boldsymbol{\sigma})$
- Rotated data points: $(\eta_0, -f_0, \varepsilon) \rightarrow (\eta, -f, \boldsymbol{K}^{\mathrm{R}}, \boldsymbol{\sigma}^{\mathrm{R}})$

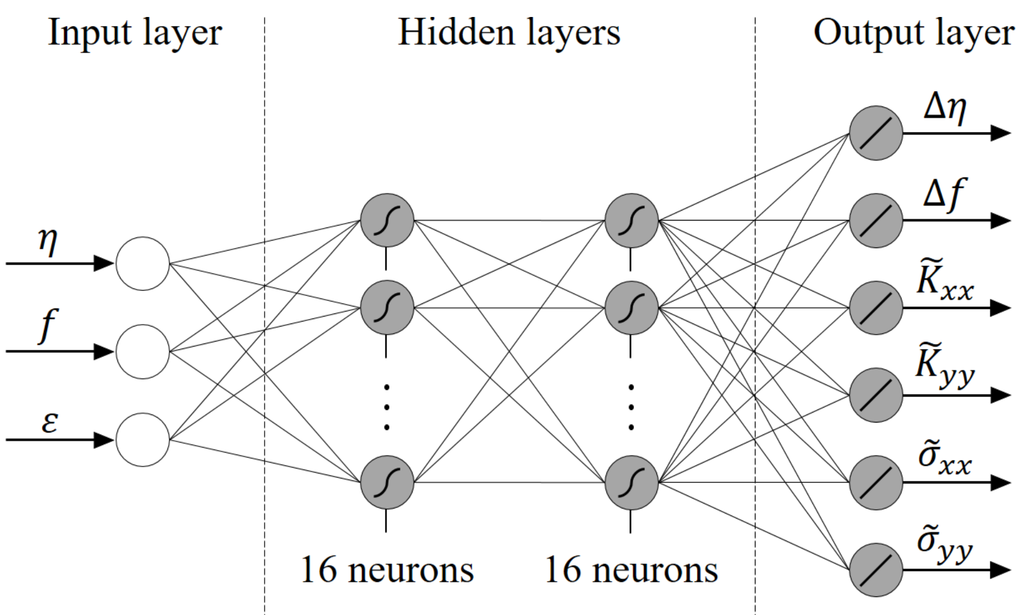
R: 90° rotation

Microscale Surrogate Model

$$(\Delta\eta, \Delta f, \widetilde{\boldsymbol{K}}, \widetilde{\boldsymbol{\sigma}}) = \psi(\eta, f, \varepsilon)$$

- **Dimensionless outputs**
  - $\widetilde{\boldsymbol{K}} = \dfrac{\boldsymbol{K}}{K}$ K: Particle conductivity
  - $\widetilde{\boldsymbol{\sigma}} = \dfrac{\boldsymbol{\sigma}}{E}$ E: Particle Young's modulus
- **Diagonal components**
  - $\widetilde{\boldsymbol{K}} = \tilde{K}_{xx}, \tilde{K}_{yy}$
  - $\widetilde{\boldsymbol{\sigma}} = \tilde{\sigma}_{xx}, \tilde{\sigma}_{yy}$

Artificial Neural Network



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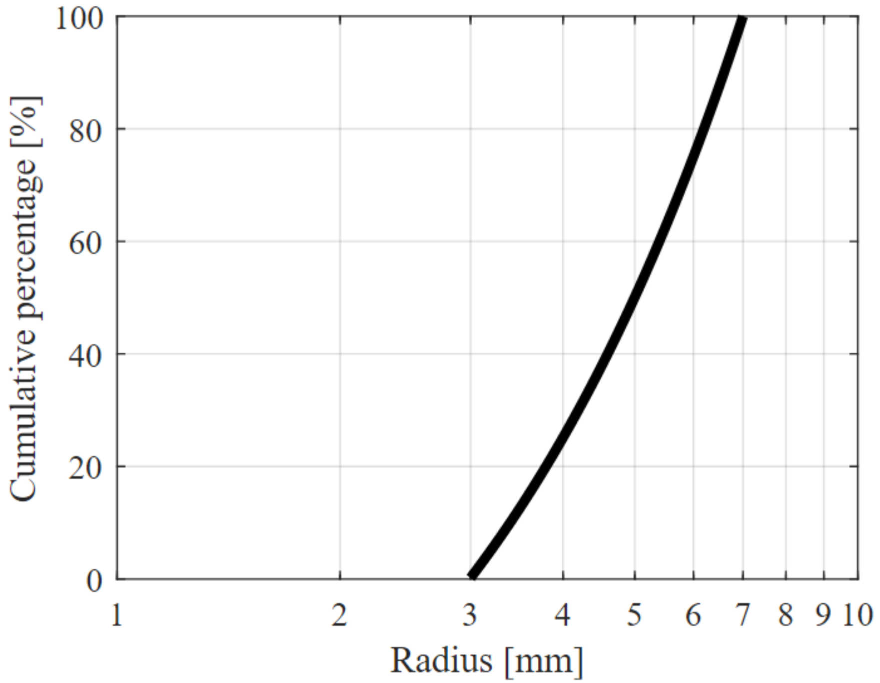
Granular Material Adopted

Particle properties

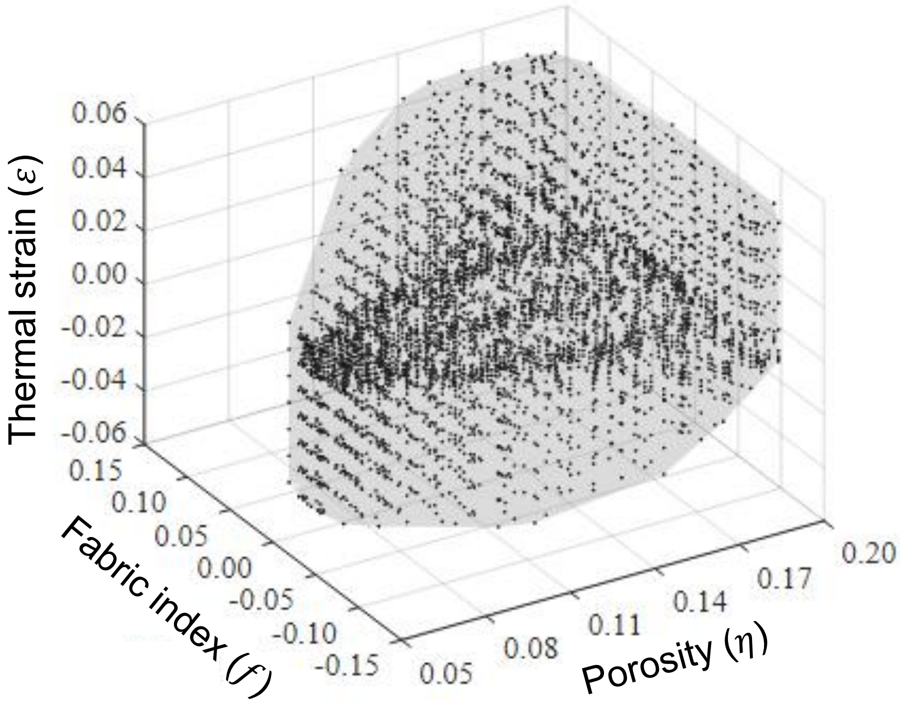
Property	Value
Density [kg/m³]	3000
Young's modulus [MPa]	10
Stiffness ratio [-]	0.8
Friction angle [-]	0.5
Thermal conductivity [W/m·K]	100
Specific heat capacity [J/kg·K]	1.0
Thermal expansion coeff. [-]	0.001
Damping coeff. [-]	0.1

Particle size distribution



Microscale Database

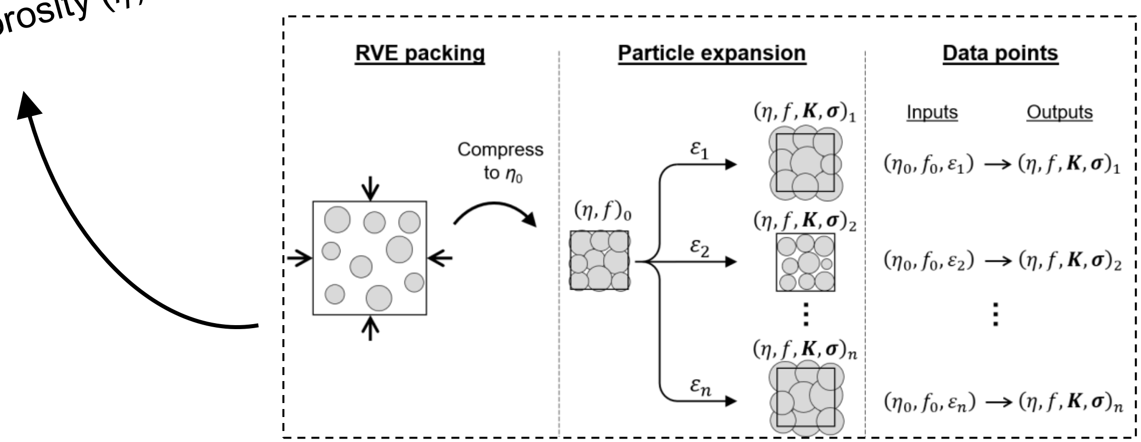
Database input space (η, f, ε)



5172 data points:

- Porosity: 6.0% – 19.5%
- Fabric: -0.14 – 0.14
- Strain: -5.0% – 5.0%

Reliable ANN prediction region (Convex hull of data points)



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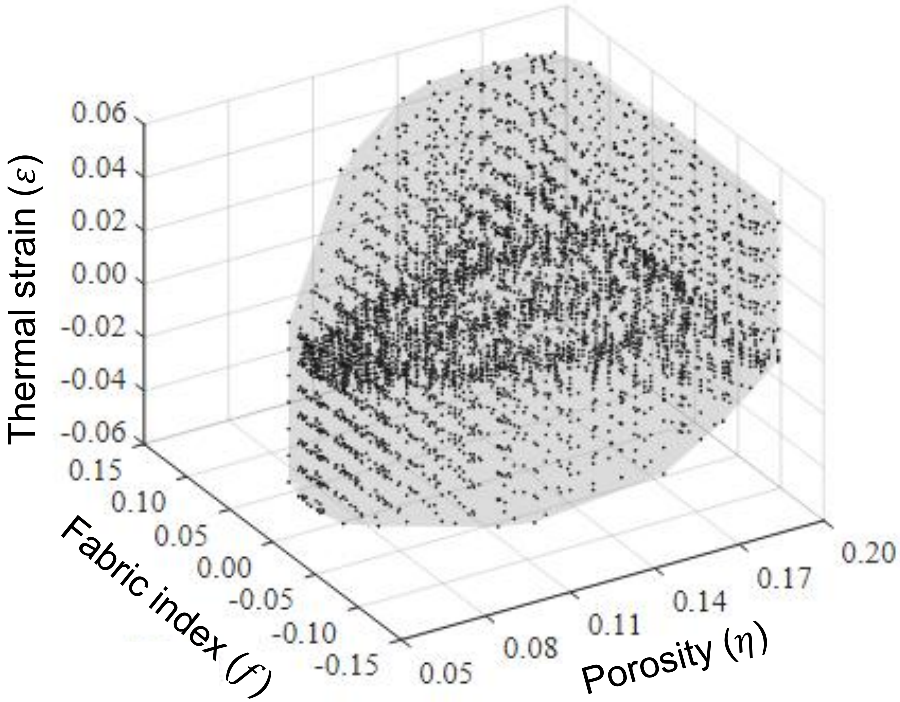

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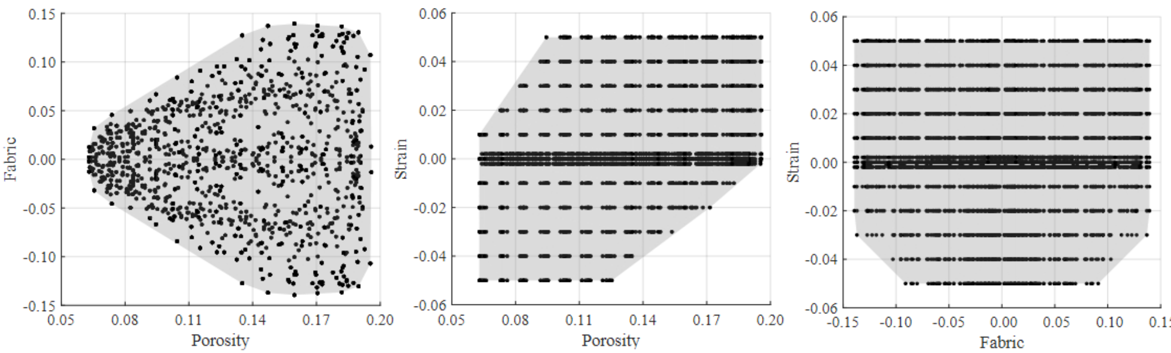
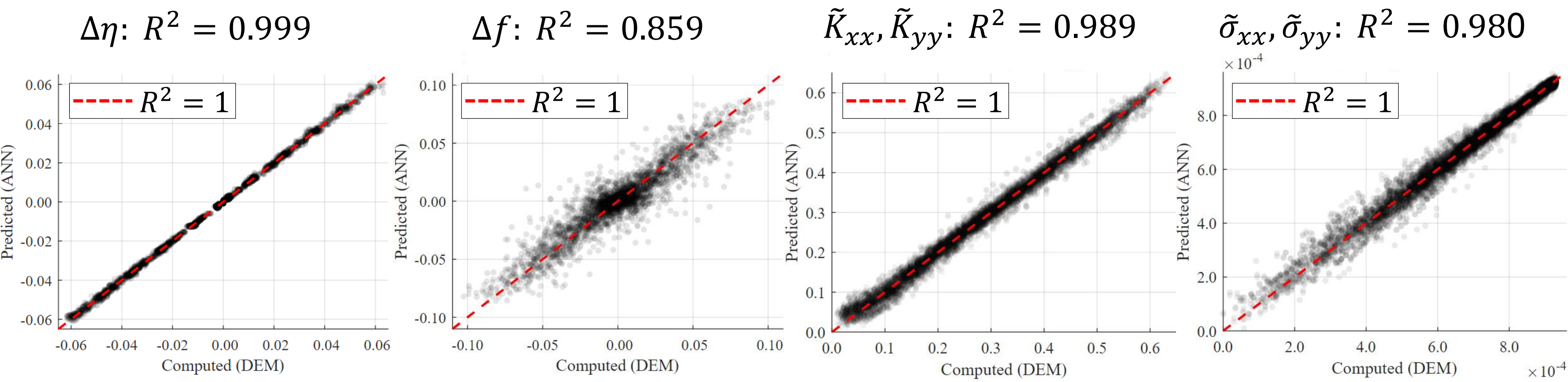


→ Higher concentration for small ε

ANN Training

Output predictions



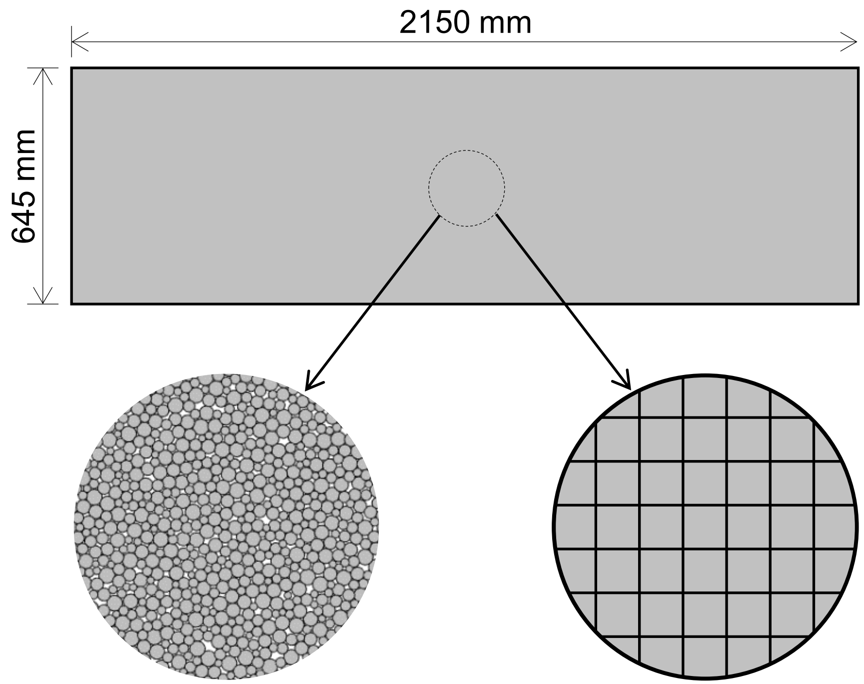
Output sensitivity to inputs

Excluded input	$\Delta\eta$	Δf	$\tilde{K}_{xx}, \tilde{K}_{yy}$	$\tilde{\sigma}_{xx}, \tilde{\sigma}_{yy}$
-	0.999	0.859	0.989	0.980
f	0.998	0.003	0.935	0.851
η	0.985	0.834	0.358	0.362
ε	0.132	0.256	0.649	0.664

No surplus or missing of important parameters!

Validation Example

Comparison between DEM and MSDD solutions



DEM model

(15000 particles)

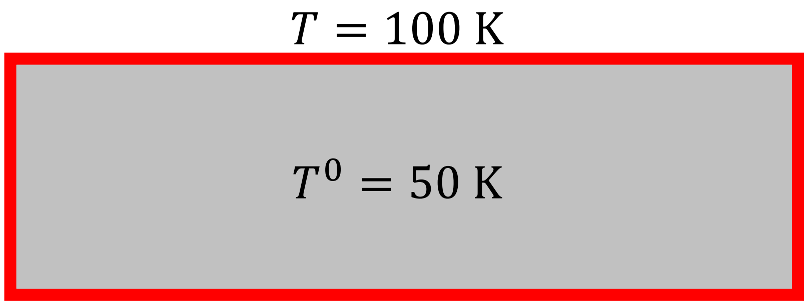
Reference solution

FVM model

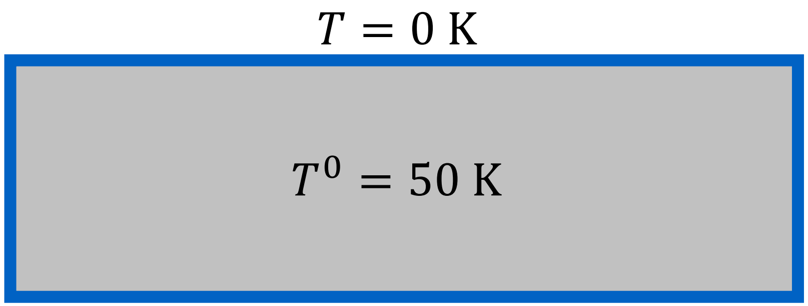
(3000 cells)

MSDD solution

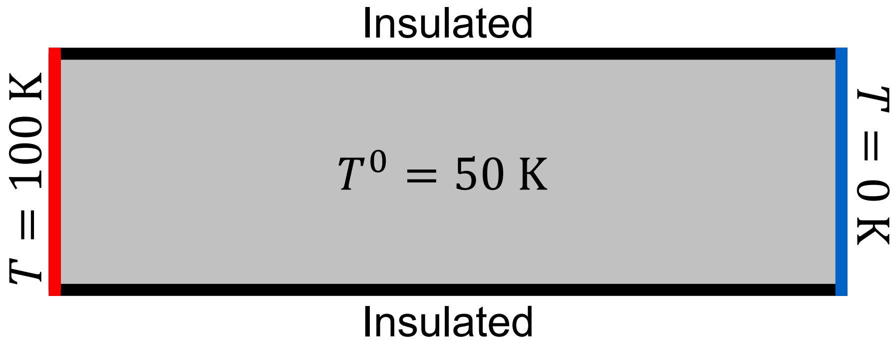
Analysis Cases



Case Hot
1. No thermal expansion (H*)
2. Thermal expansion (H)



Case Cold
3. No thermal expansion (C*)
4. Thermal expansion (C)

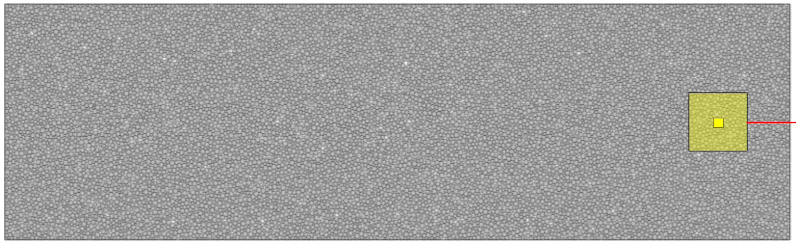


Case Hot-Cold
5. No thermal expansion (HC*)
6. Thermal expansion (HC)

Initial Conditions for MSDD Solution

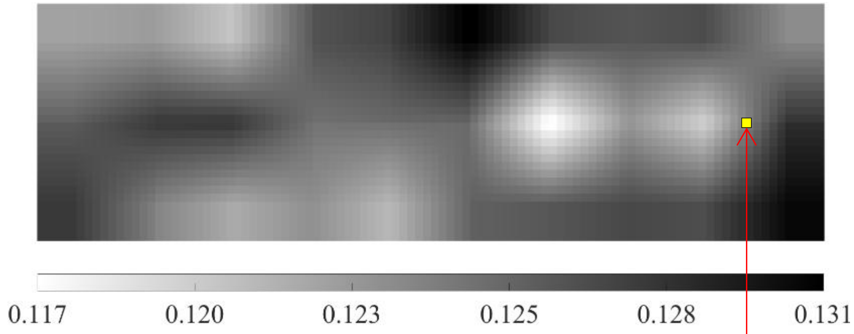
Reference DEM model

Properties calculated locally around each FVM cell centroid

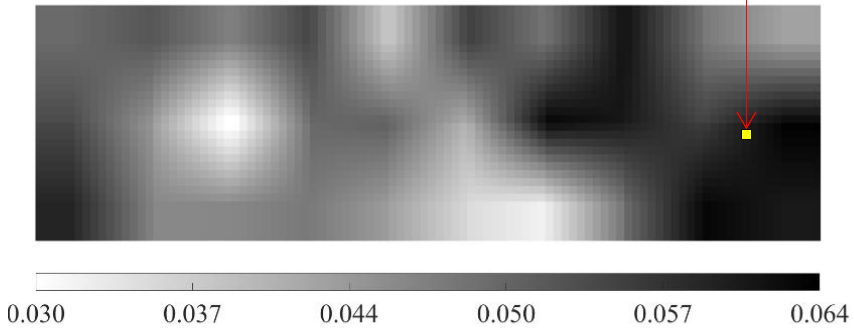


FVM model for MSDD

Local porosities (η)

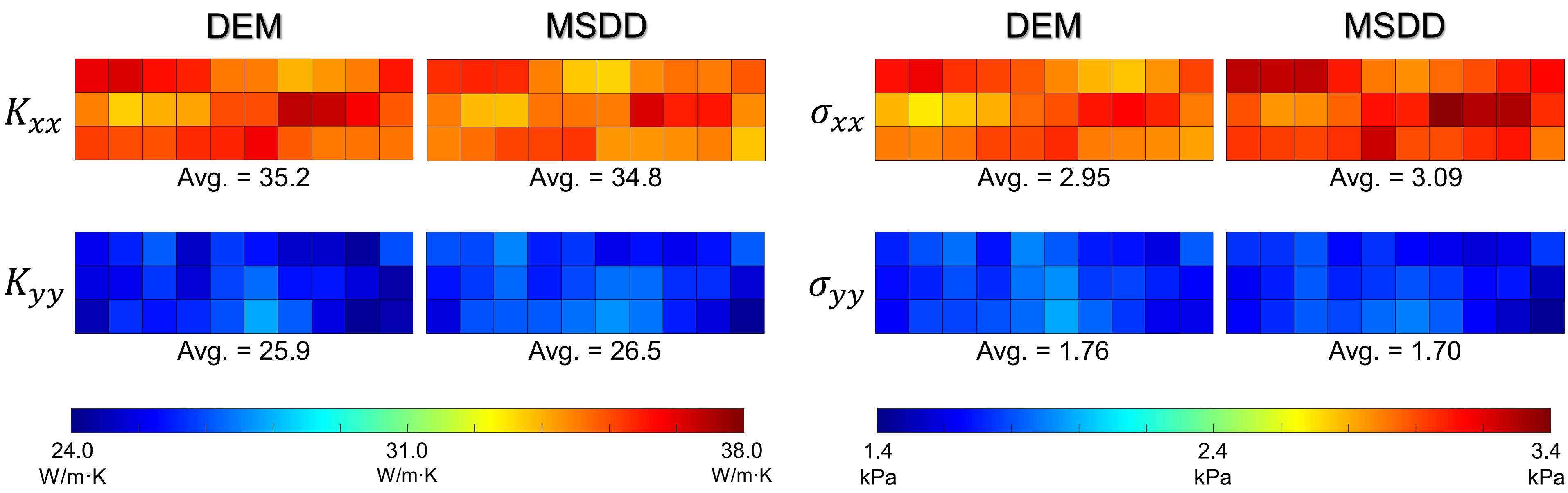


Local fabric indexes (f)



Results Without Thermal Expansion

Thermal conductivity distribution | **Cauchy stress distribution**

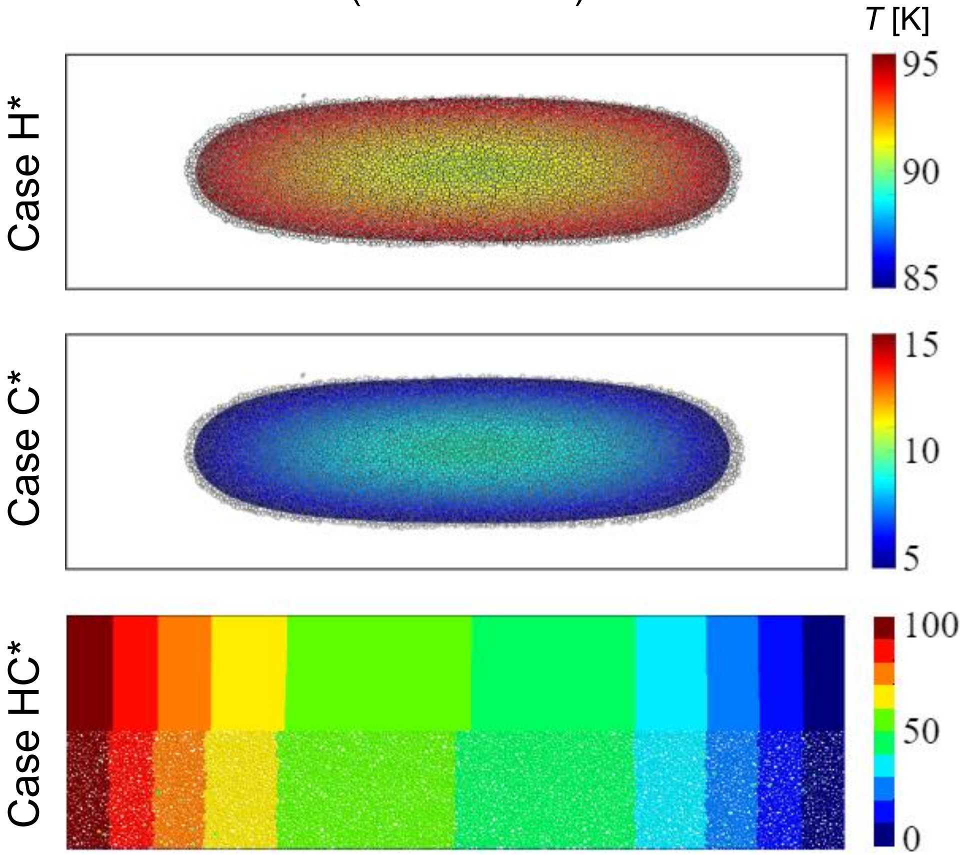


Purely thermal analysis: static microstructure.

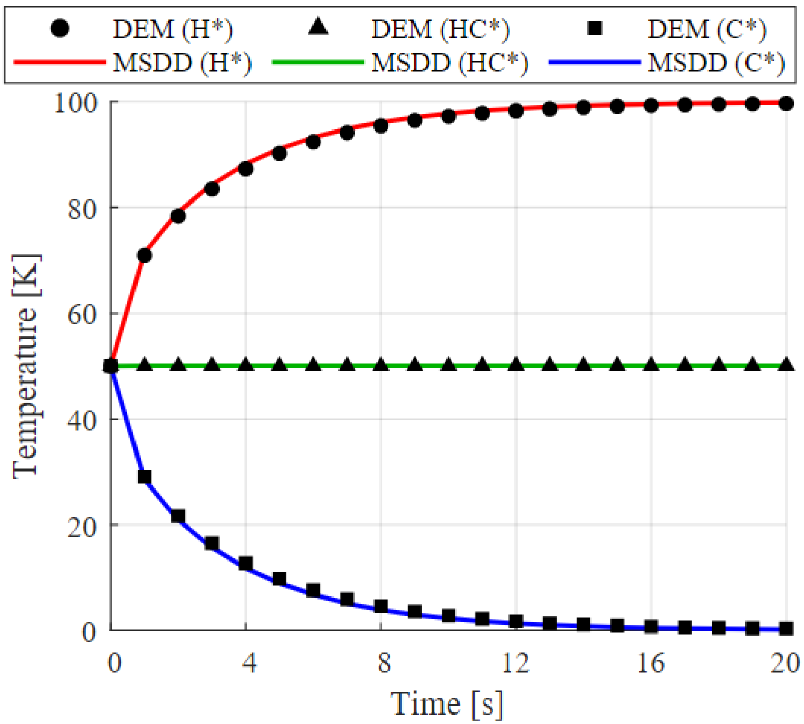
Good predictions of $\boldsymbol{K}$ and $\boldsymbol{\sigma}$ from porosity and fabric.

Results Without Thermal Expansion

Temperature contours
(at 8 seconds)



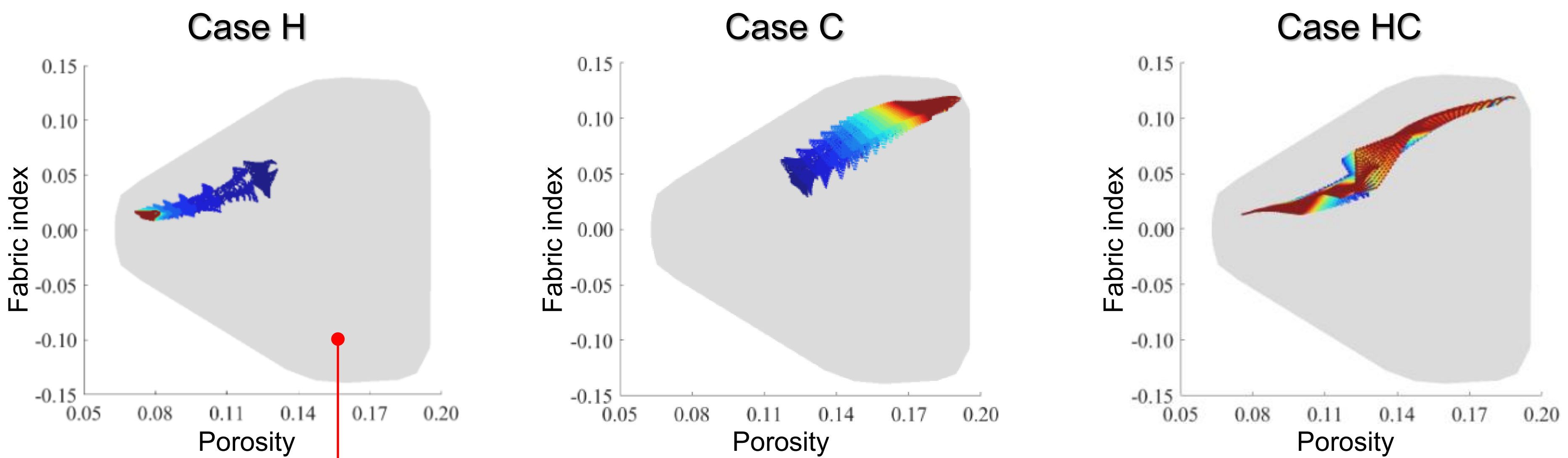
Average temperature evolution



Results With Thermal Expansion

Transient response

Evolution of input parameters (η, f) in the MSDD solution

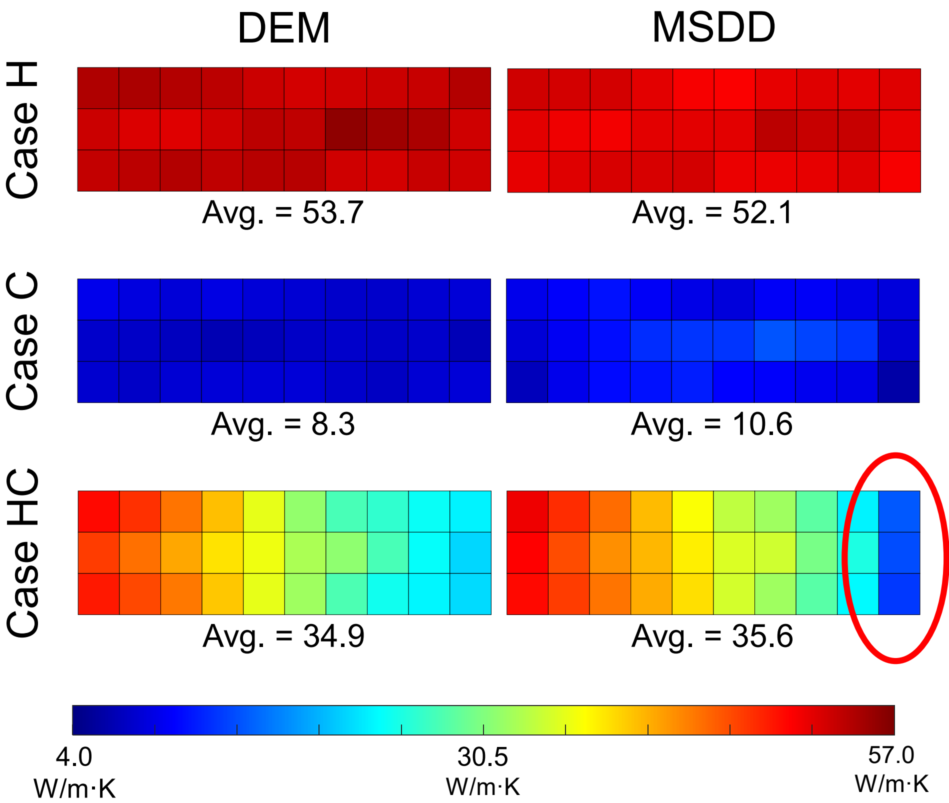


Reliable ANN prediction region ($\eta \times f$ plane)

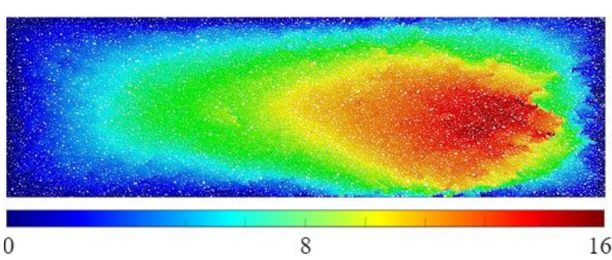
No extrapolation by the surrogate model!

Results With Thermal Expansion

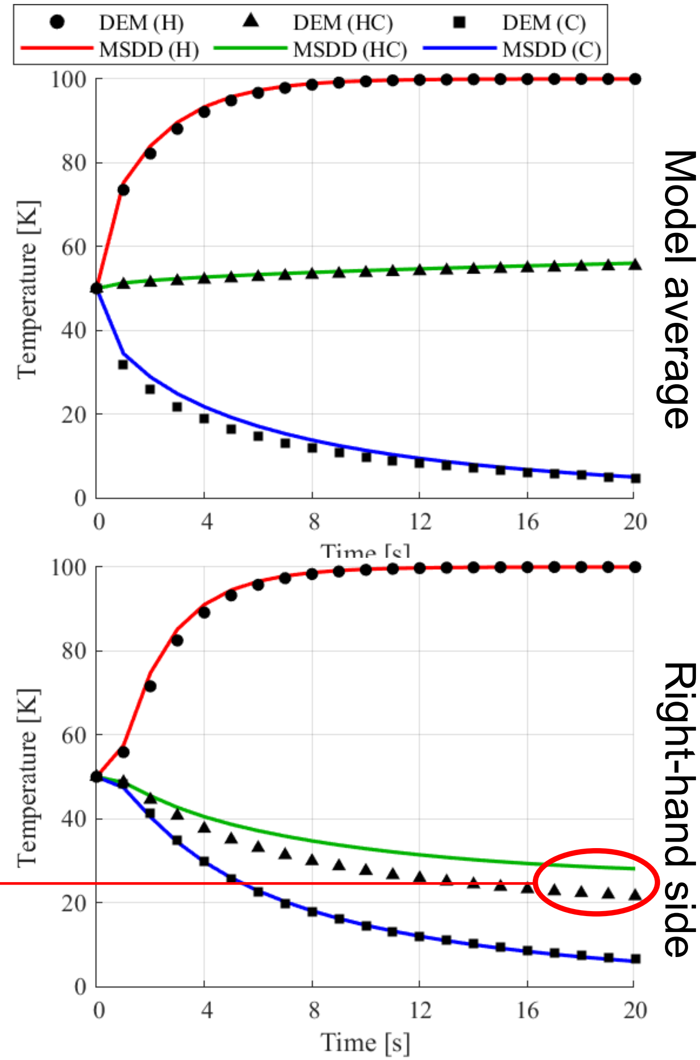
Final thermal conductivity distribution K_{xx}



Bulk motion: final particle displacements

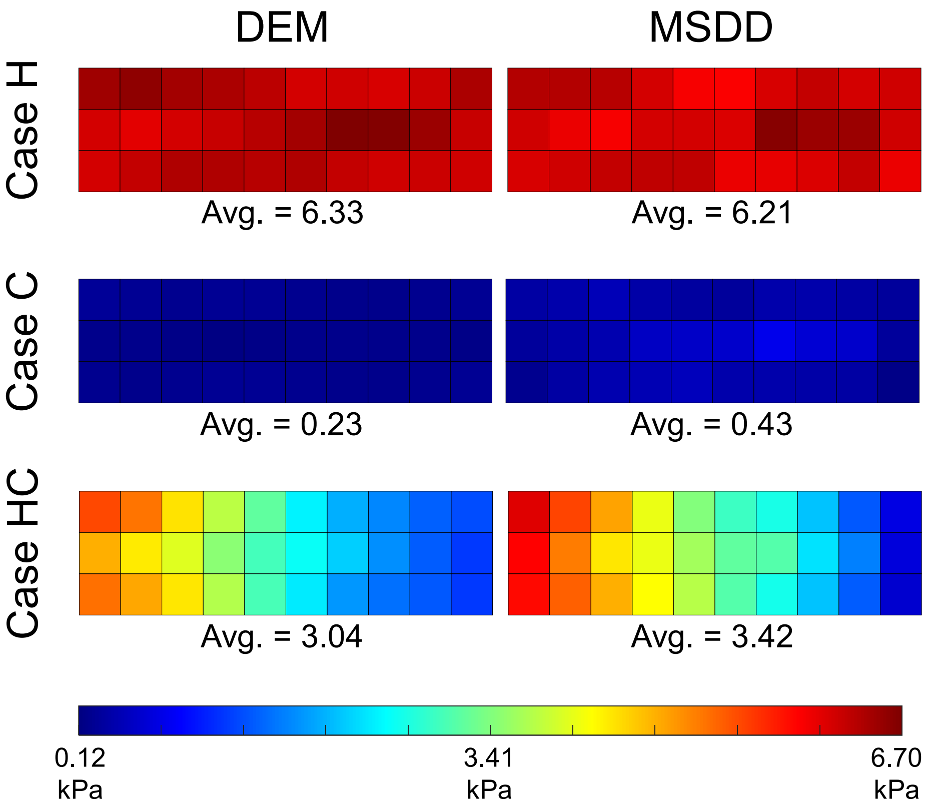


Temperature evolution



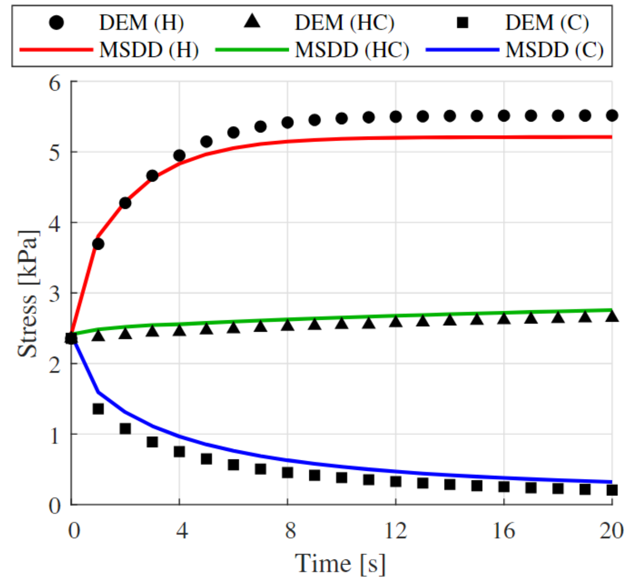
Results With Thermal Expansion

Final Cauchy stress distribution σ_{xx}



Average effective stress evolution

$$p = \frac{\sigma_{xx} + \sigma_{yy}}{2}$$

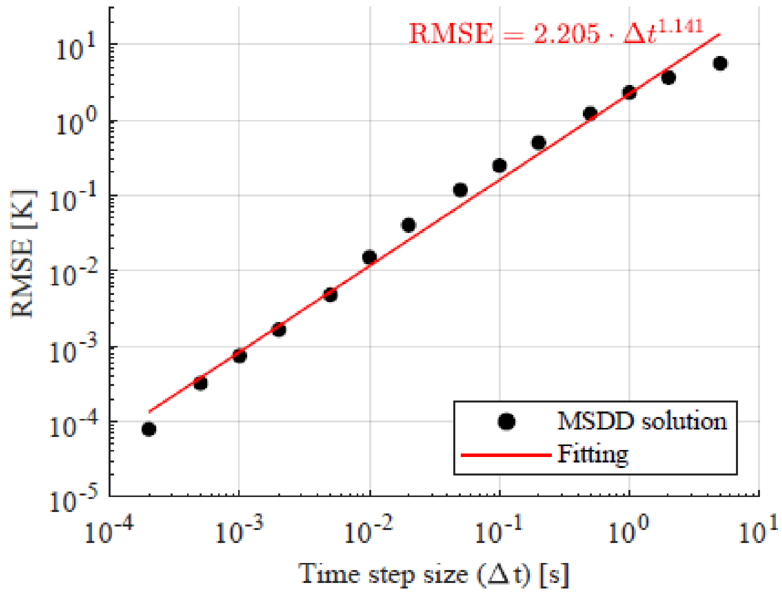


Results With Thermal Expansion

Convergence analyses of MSDD solution

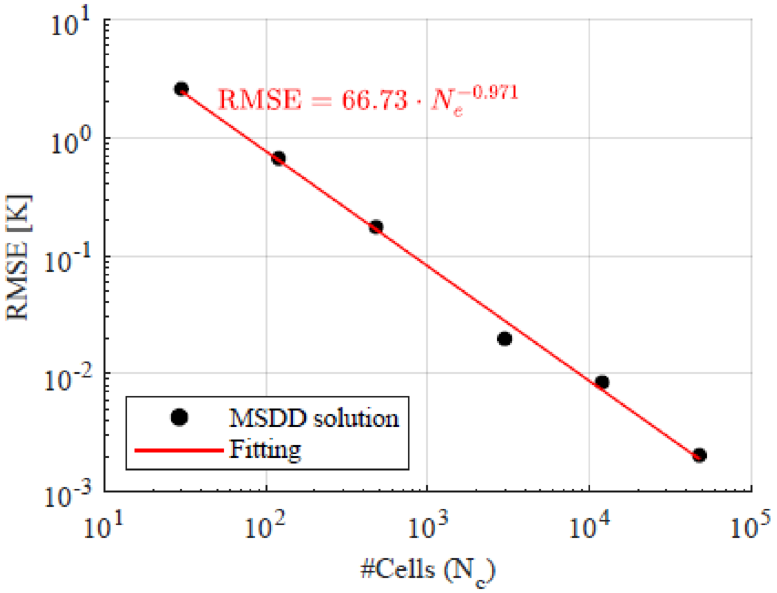
Time step size

(RMSE for avg. temperature in case H)



FVM mesh refinement

(RMSE for avg. temperature in case H)



Results With Thermal Expansion

Simulation Elapsed Times

Analysis case	DEM wall-clock time [s]	MSDD wall-clock time [s] *	DEM / MSDD speedup factor
H	112,054		2.7×10^3
C	78,551	41	1.9×10^3
HC	96,591		2.4×10^3

* Online macroscale solution only

1 – Introduction

2 – Methodology

3 – Results and Discussions

4 – Conclusions

Conclusions

Main achievements

- An online-offline approach based on machine-learning for hierarchical multiscale modeling.
- Transient analyses of thermal expansion and conduction in confined granular media.
- Validation results show:
  - Accuracy comparable to DEM.
  - Efficiency of a continuous method.

Main limitations

- Database generation cost:
  Several RVE simulations for each particular problem.
- Microscale representativeness:
  Variability of microscale response in RVEs with similar configurations.
- ANN fitting errors:
  Influence of neglected input parameters.
- Bulk granular motion:
  Mass / size conserving RVEs cannot account for global particle displacements.

Future Work

- Extend to 3D.
- Surrogate model generalization:
  Different particle size distributions, etc.
- Extend thermal behavior:
  Different heat transfer mechanisms and models.
- Add mechanical behavior:
  Solve equilibrium equation at the macroscale: larger deformation problems
- Apply to real-world problems:
  Thermal cycling, granular flows, etc.

THANK YOU

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