THM short-course: Day 3

ThermalEngine - THM coupling

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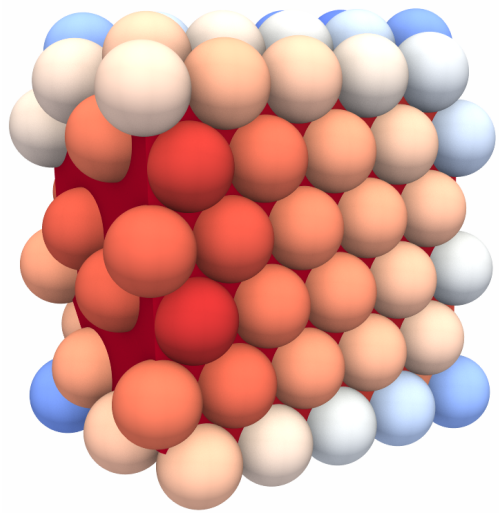
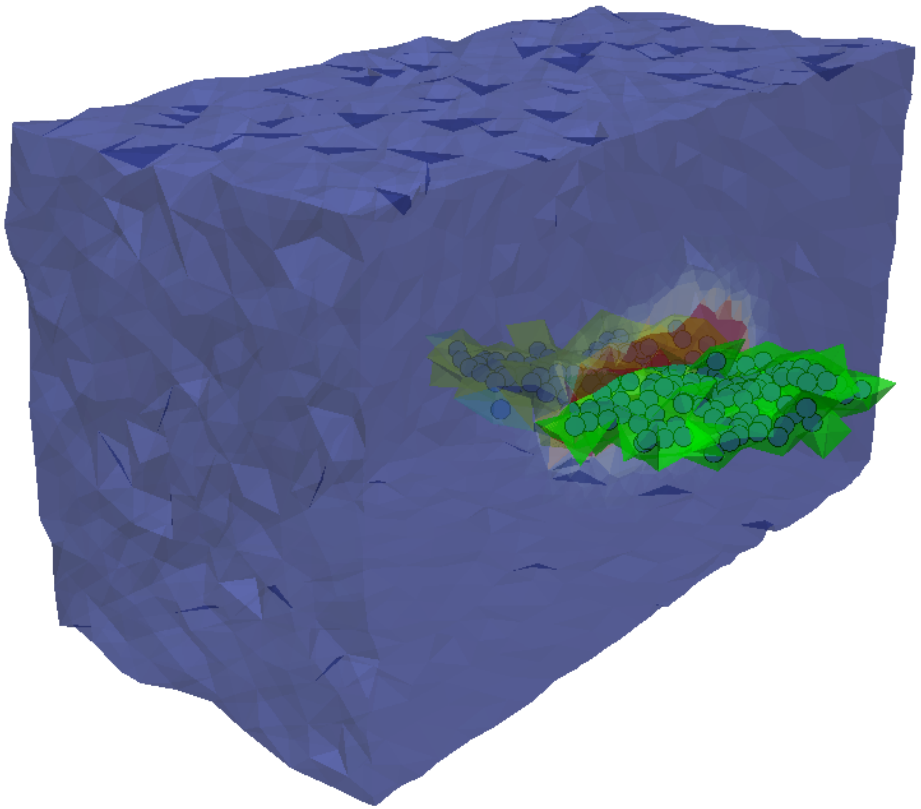


Why?

Geomechanical thermo-hydro-mechanical failure simulations can exploit:

(1) Explicit discontinuous methods (Yade, DEM)
(2) Implicit stoke's-flow coupling (Pore Finite Volume method)
(3) Complementary heat advection and well established particle heat conduction (`ThermalEngine`)



Framework overview

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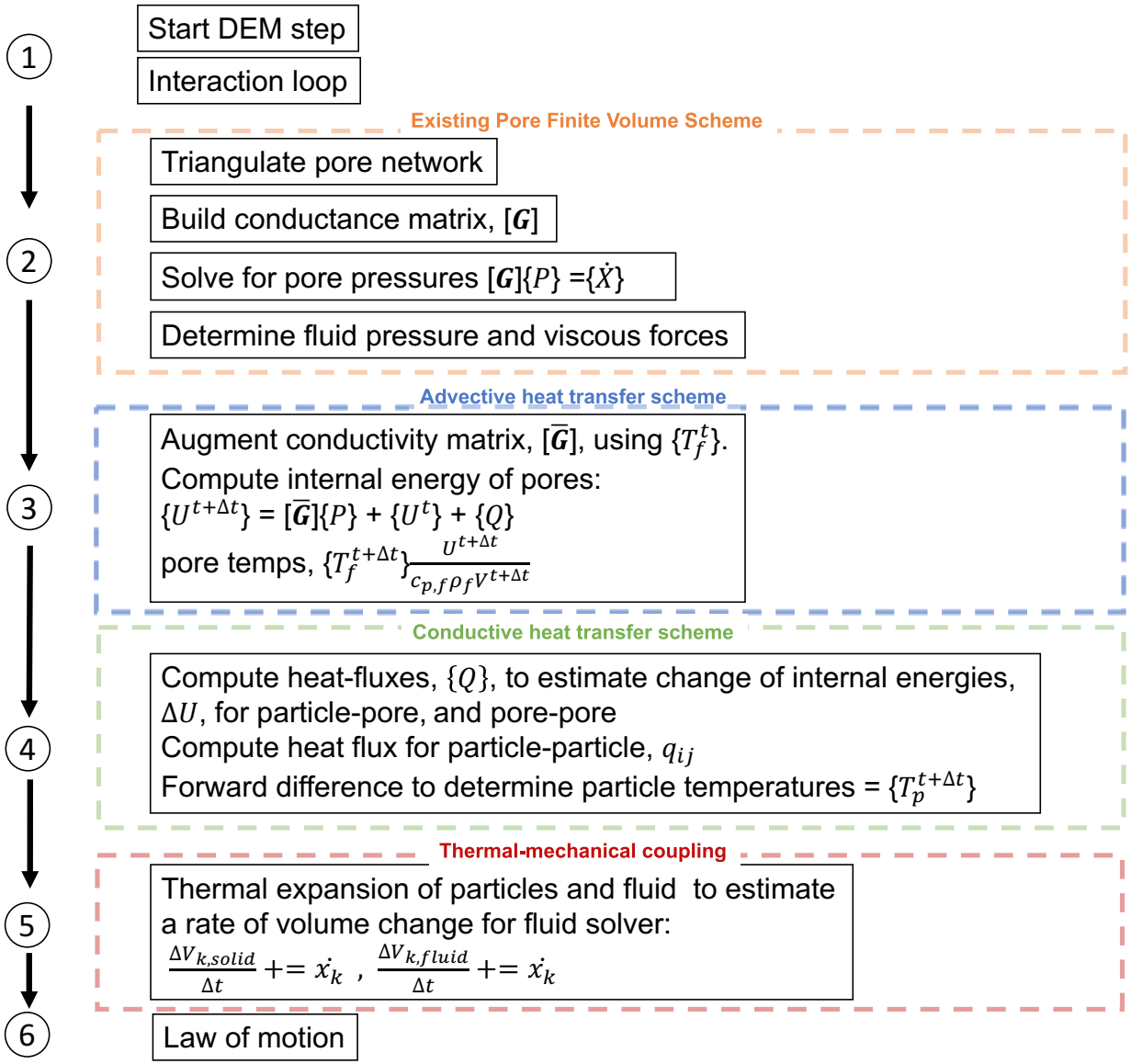

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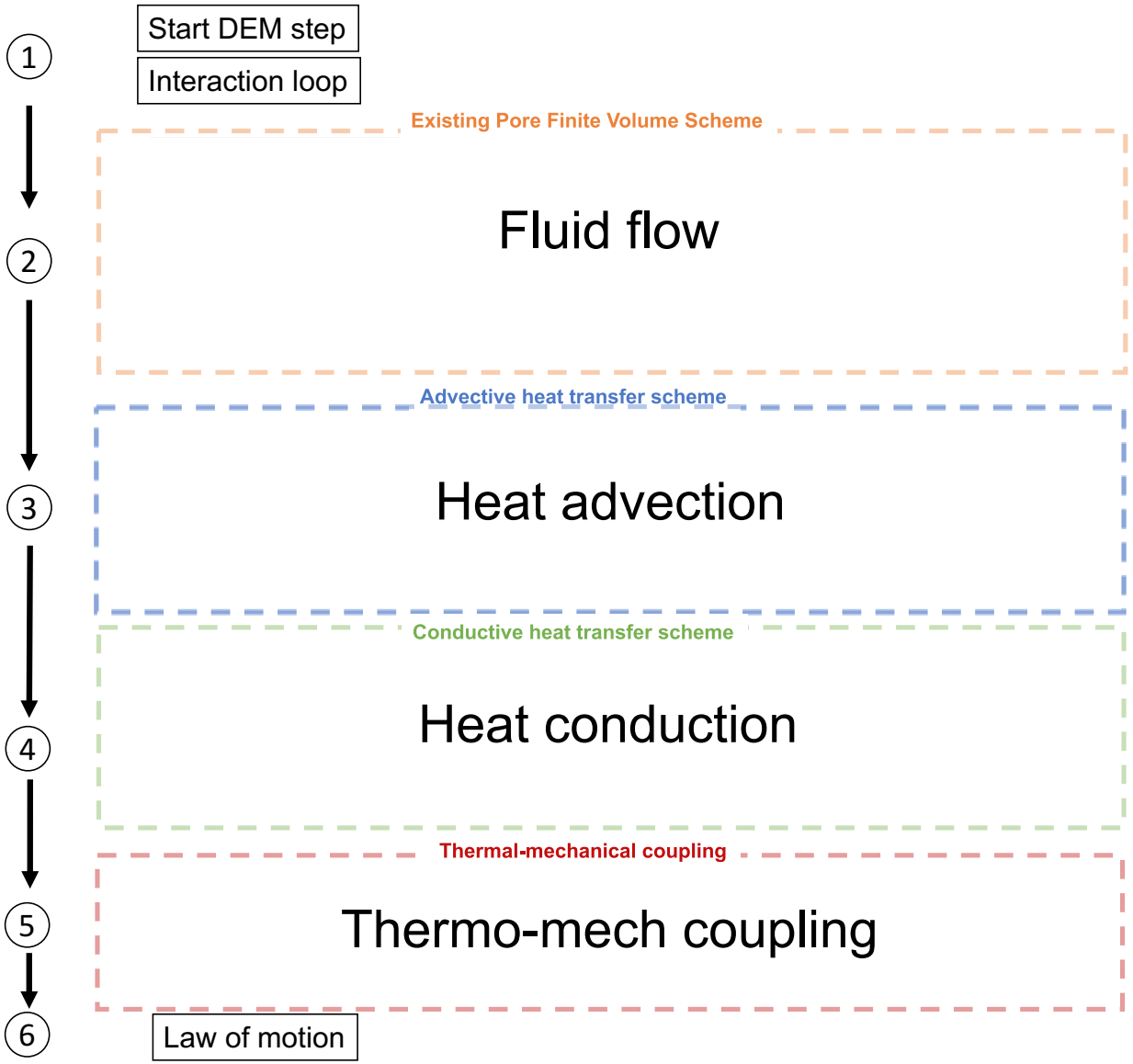

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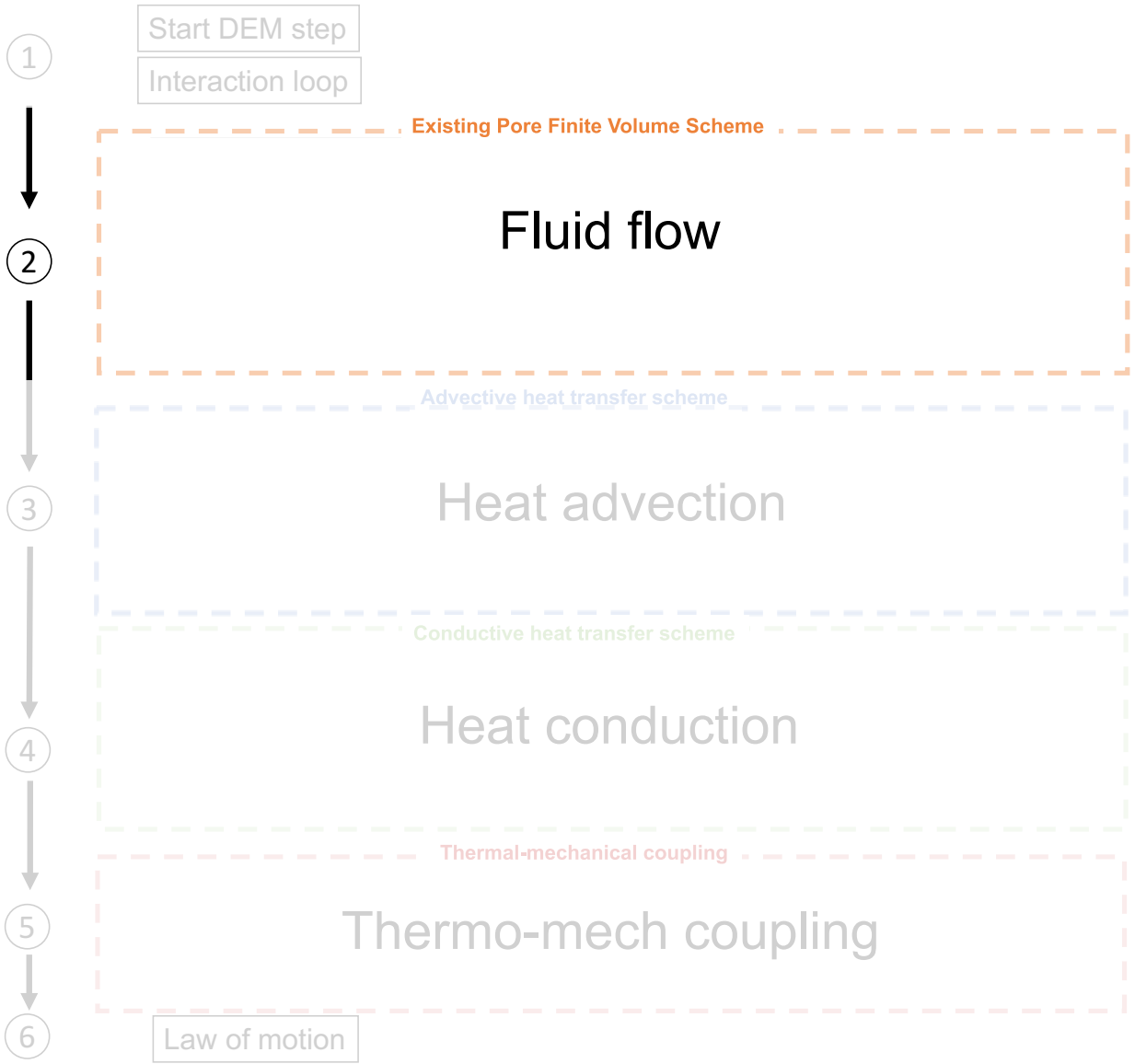


Pore Finite Volume scheme

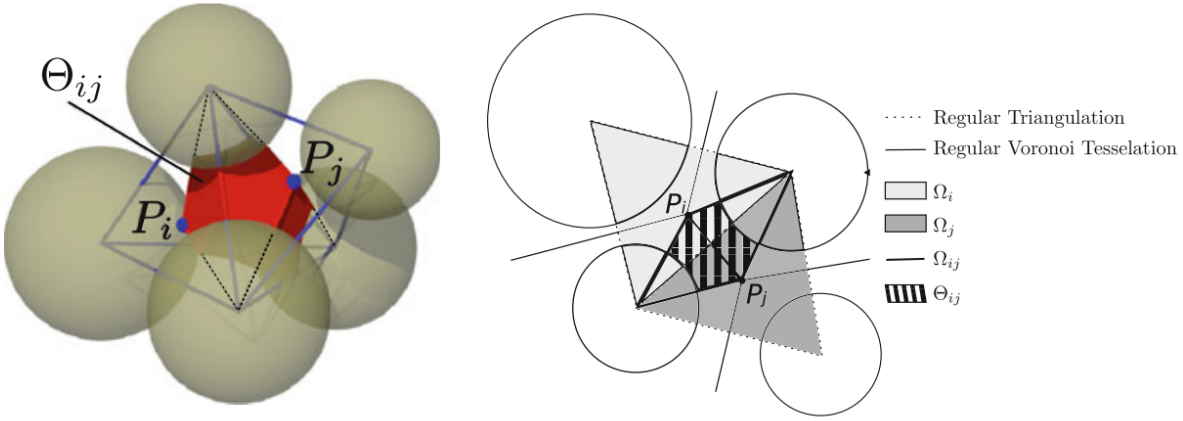


Figure 1: Triangulation of pore space and connecting pore throats in sphere packing [2]

Pore Finite Volume scheme

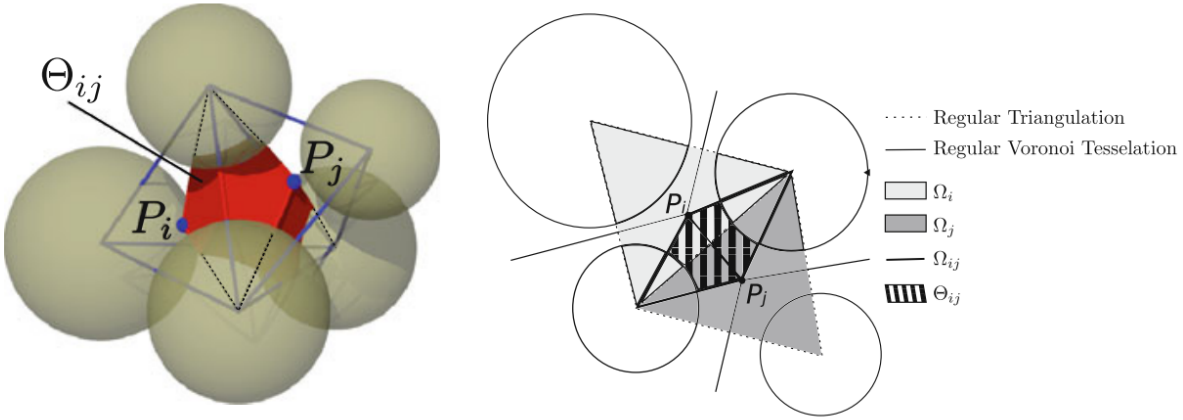


Figure 1: Triangulation of pore space and connecting pore throats in sphere packing [2]

Continuity equation:

$$\int_{\Theta_i} \frac{1}{K} \frac{\partial p_i}{\partial t} = \int_{\partial\Theta_i} (\mathbf{u} - \mathbf{v}) \cdot \mathbf{n} \, \mathrm{d}S - \dot{V}_{p,i} \tag{1}$$

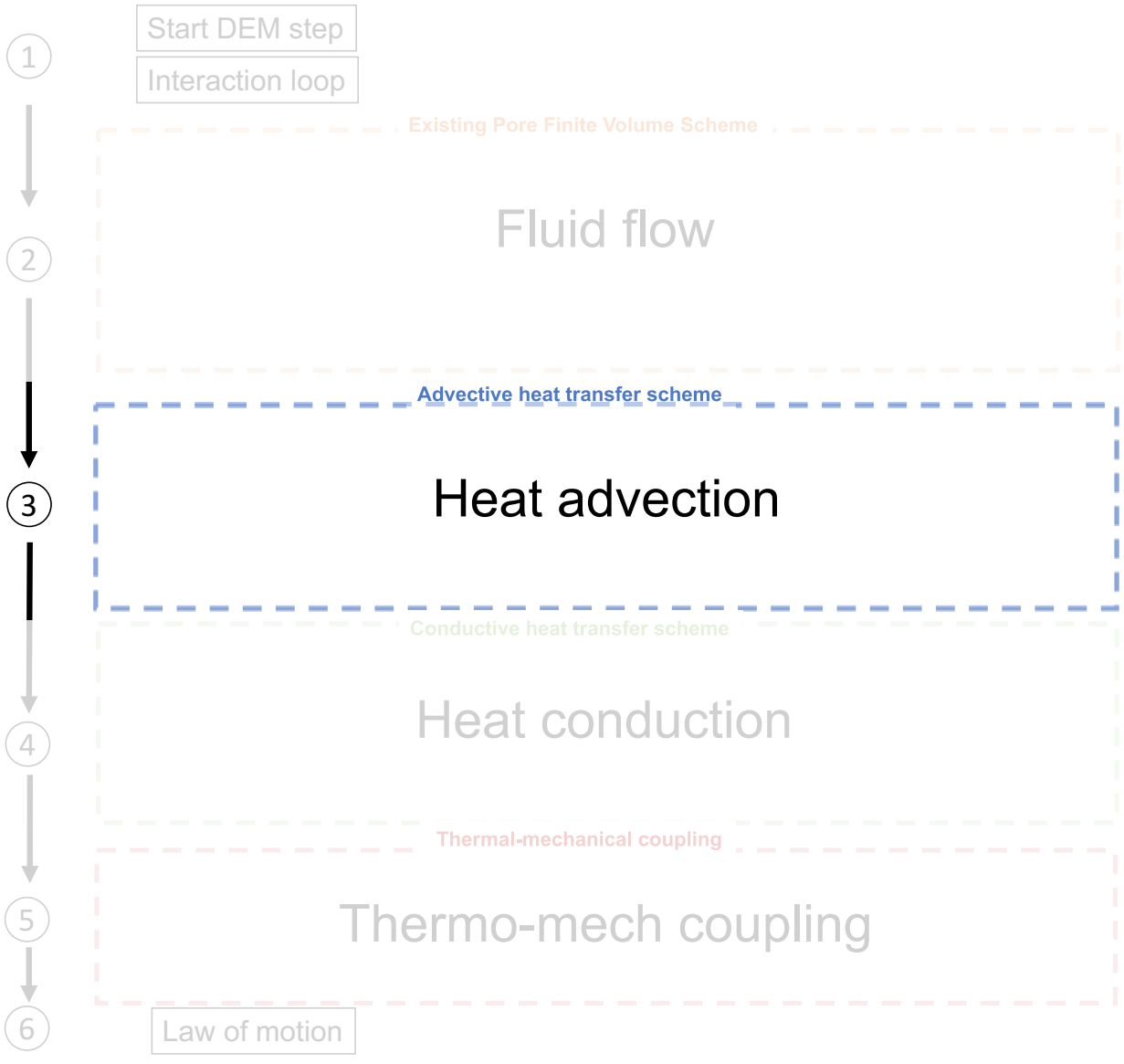
$$q_{ij} = k_{ij} \frac{p_i - p_j}{l_{ij}} \tag{2}$$

$$\sum_{j=1}^{4} q_{ij} = \dot{V}_{p,i} + \frac{\dot{p}_i V_{p,i}}{K} \tag{3}$$

Implicit formulation:

$$\mathbf{G}\mathbf{p} = \mathbf{E}\dot{\mathbf{x}} \tag{4}$$

Framework overview



Advective heat transfer

Pores treated as open thermodynamic systems:

$$\Delta U = Q + W + \Delta U_{matter} \tag{5}$$

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$$[\bar{\mathbf{G}}] = c_{p,f} \rho_f \Delta t \sum_{j=1}^{4} T^t_{(i \text{ or } j)} g_{ij}. \tag{7}$$

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is multiplied by the PFV pressure field to determine the internal energy field:

$$\{\mathbf{U^{t+\Delta t}}\} = [\bar{\mathbf{G}}]\{\mathbf{p}\} + \{\mathbf{U^t}\} + \{\mathbf{\Phi}\}\Delta t \tag{8}$$

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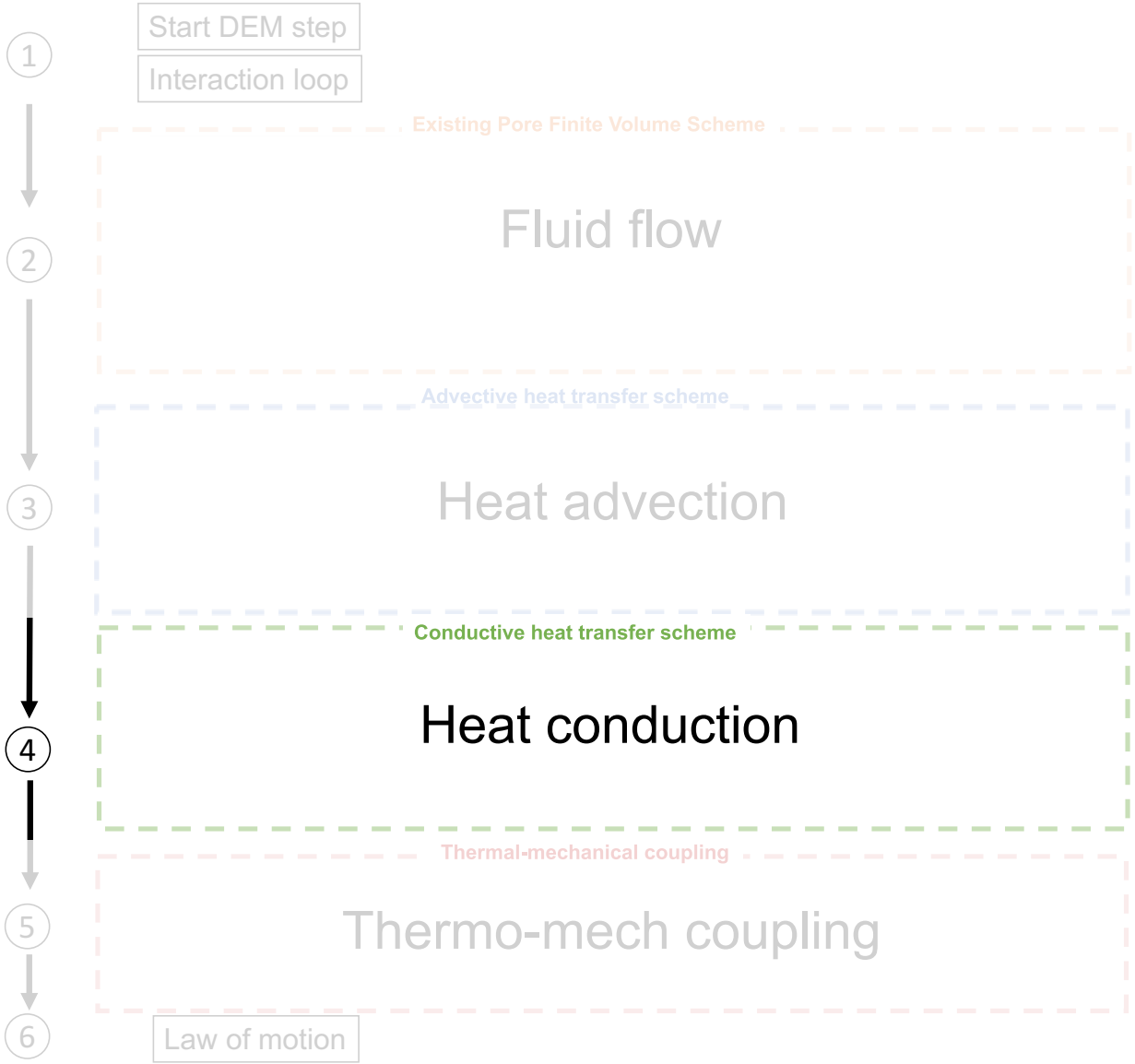
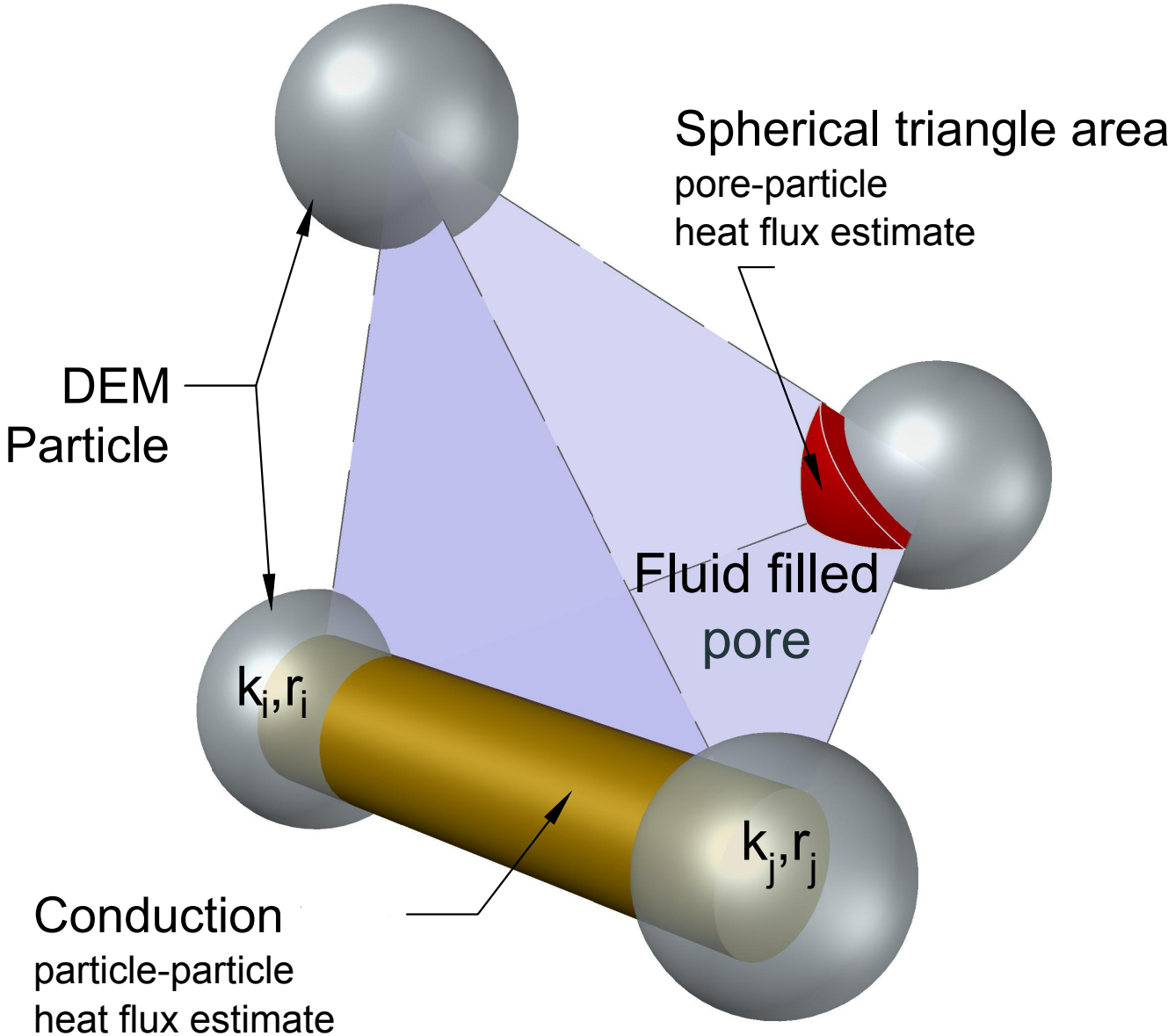


Conductive heat transfer



Conductive heat transfer

Conservation of energy per particle [6]:

$$m_i c_{p,i} \frac{\mathrm{d}T_i}{\mathrm{d}t} = \sum_{j=1}^{N} \Phi_{i,j} + \sum_{k=1}^{M} \Phi_{i,k} \tag{9}$$

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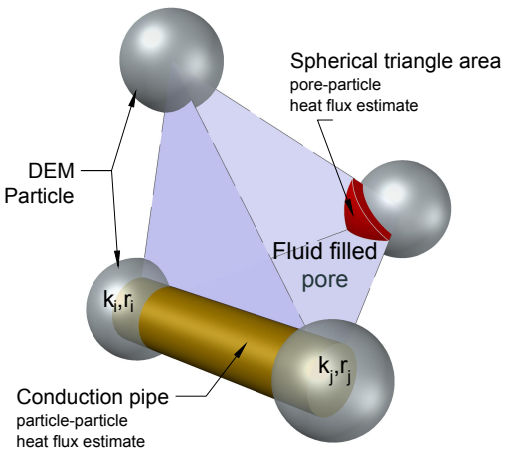
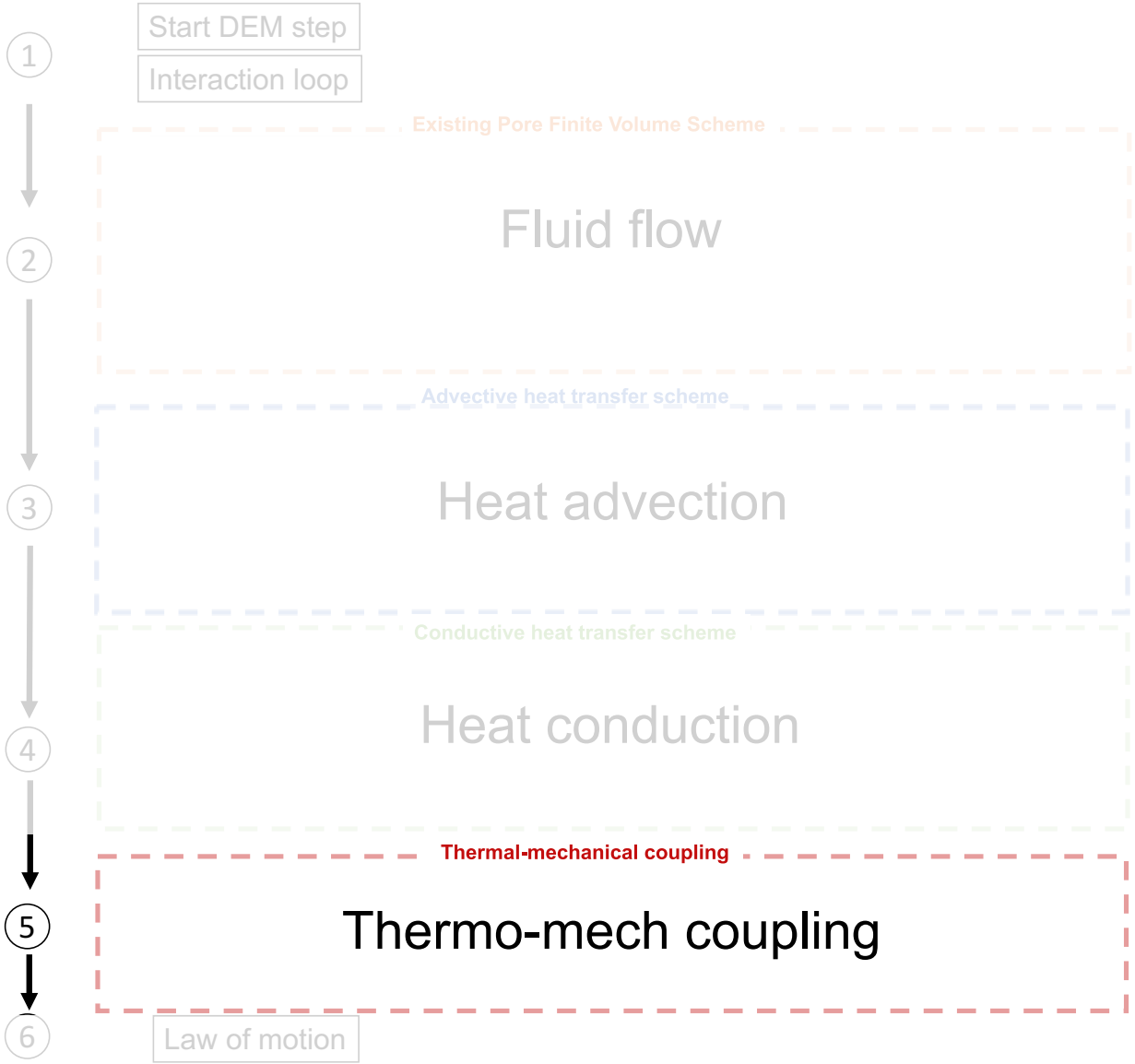
$$\Phi_{i,j} = \frac{2r_c^2(k_i + k_j)}{d}(T_j - T_i) \tag{10}$$

Particle→Pore [5]:



$$\Phi_{i,k} = h_i A_i (T_k - T_i) \tag{11}$$

Framework overview



Thermo-Mechanical coupling

Particle thermal expansion(contraction):

$$\Delta r_i^{t+\Delta t} = r_i^t \beta_p (T_i^{t+\Delta t} - T_i^t) \tag{12}$$

$$\Delta v_k = -\sum_{i=1}^{4} \frac{A_{sph,i}}{A_{tot,i}} \frac{4}{3} \pi (r_{i,t+\delta t}^3 - r_{i,t}^3) \tag{13}$$

$$E\dot{x}_k \mathrel{+}= \frac{\Delta v_k}{\Delta t} \tag{14}$$

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Pore fluid thermal expansion(contraction):

$$E\dot{x}_k \mathrel{+}= \frac{V_k \beta_f \Delta T}{\Delta t} \tag{15}$$

Hydro-Mechanical Coupling

Pressure force:

$$\mathbf{F_{ij}^{p,k}} = A_{ij}^{k}(p_i - p_j)\mathbf{n}_{ij} \qquad (16)$$

Viscous force:

$$\mathbf{F_{ij}^{V}} = A_{ij}^{f}(p_i - p_j)\mathbf{n}_{ij} \qquad (17)$$

$$\mathbf{F_{ij}^{v,k}} = \mathbf{F_{ij}^{V}} \frac{\gamma_{ij}^{k}}{\sum_{k=1}^{3} \gamma_{ij}^{k}} \qquad (18)$$

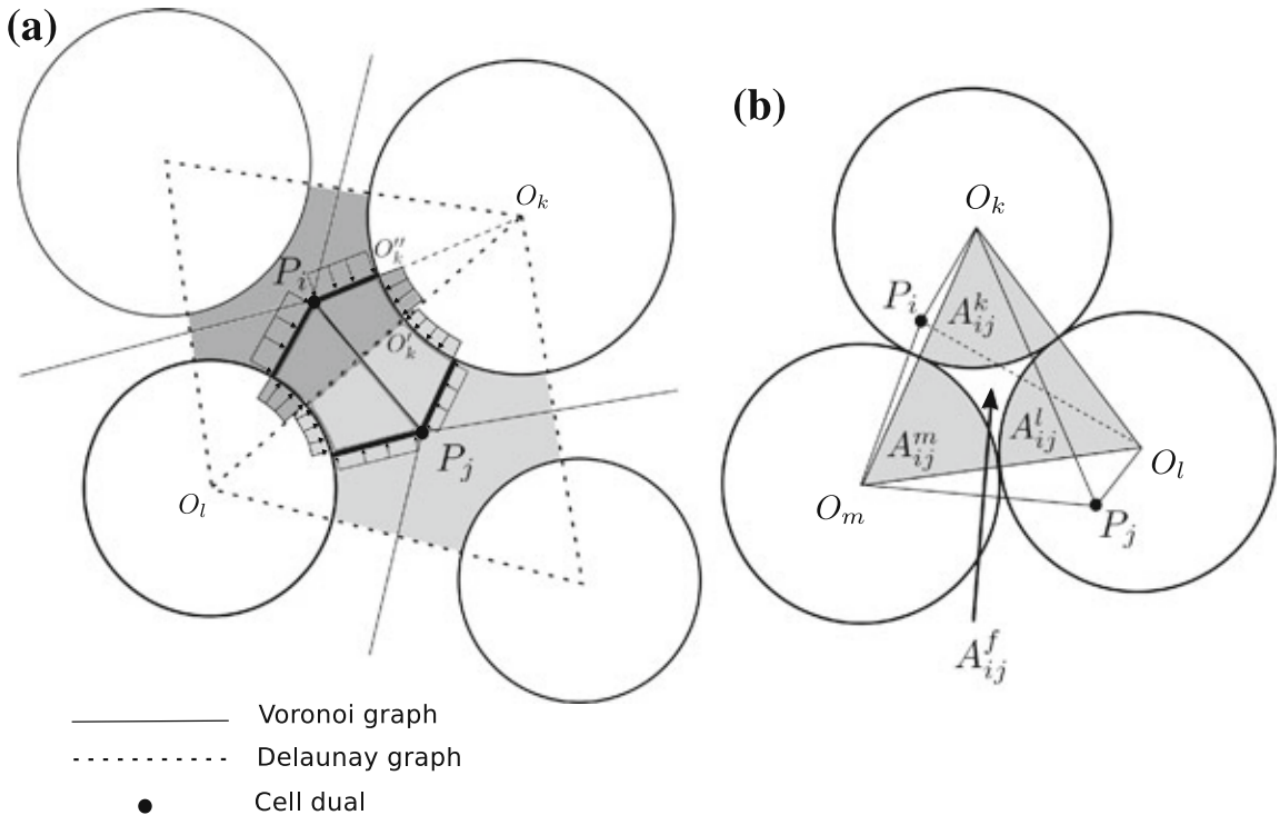


Figure 2: Pore volume decomposition for pressure and viscous forces [2].

Validation

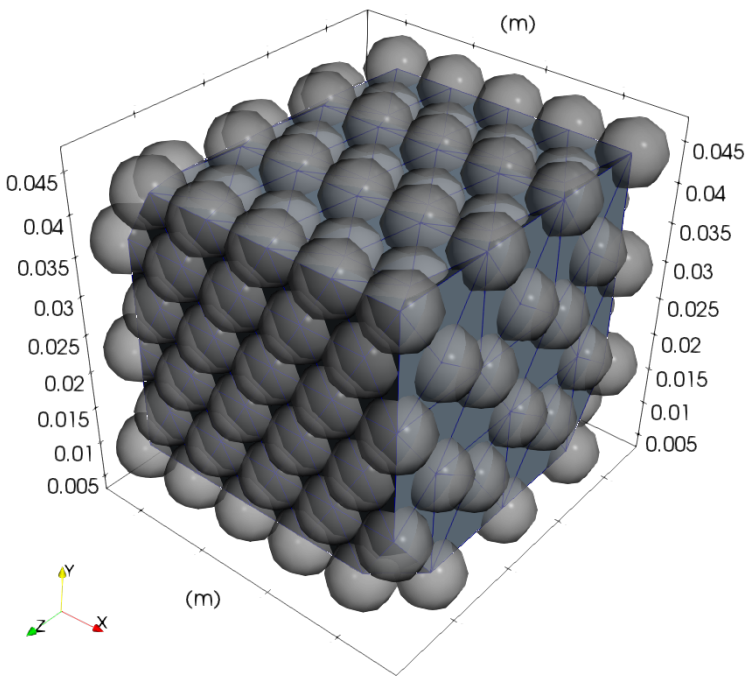
Numerical validation: ANSYS CFX vs Yade DEM

Identical sphere packings, solid and fluid parameters, boundary conditions, and durations:

(1) No-flow: pressure gradient of 0 pa, hot water transfers heat to cool sphere packing

(2) Flow: pressure gradient of 10 pa, flush hot water through cool sphere packing

Yade DEM



ANSYS CFX

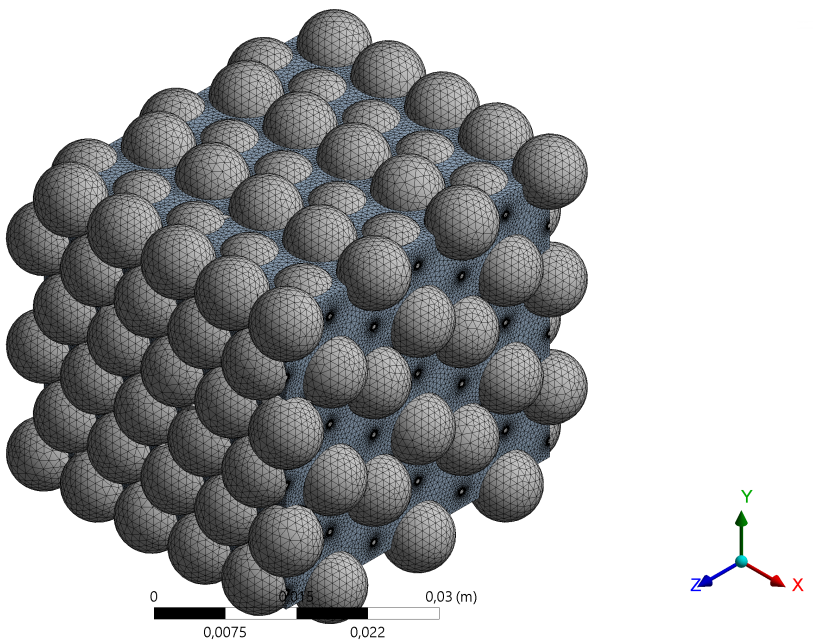


Figure 3: left) DEM Yade sphere packing and pore network right) ANSYS CFX mesh

Numerical validation: No-Flow condition

Still water at 70°C transferring heat to 60°C sphere packing:

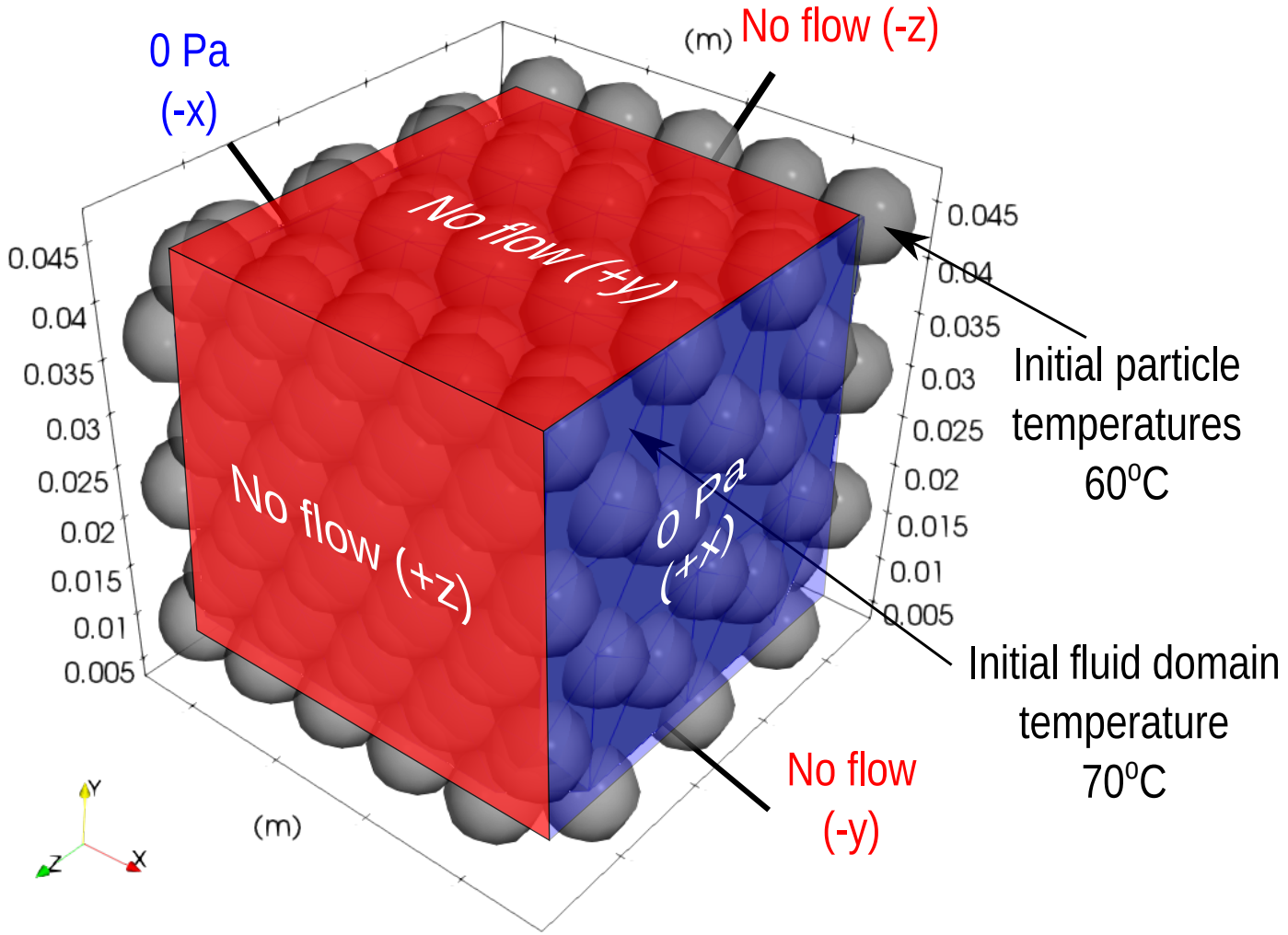


Figure 4: Specimen dimensions and boundary conditions for Yade DEM and ANSYS CFX No-Flow scenario.

Numerical validation: No-Flow condition

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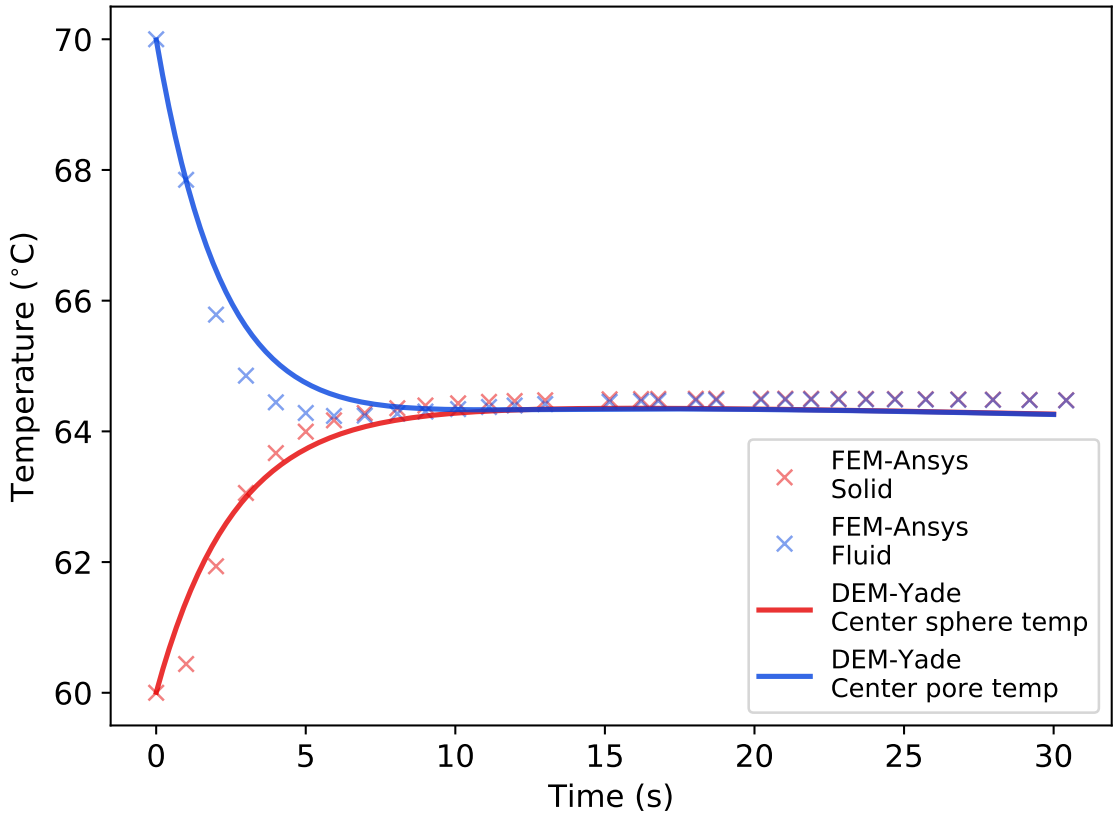


Figure 5: Center body and pore temperature comparison for Yade and ANSYS.

Numerical validation: No-Flow condition

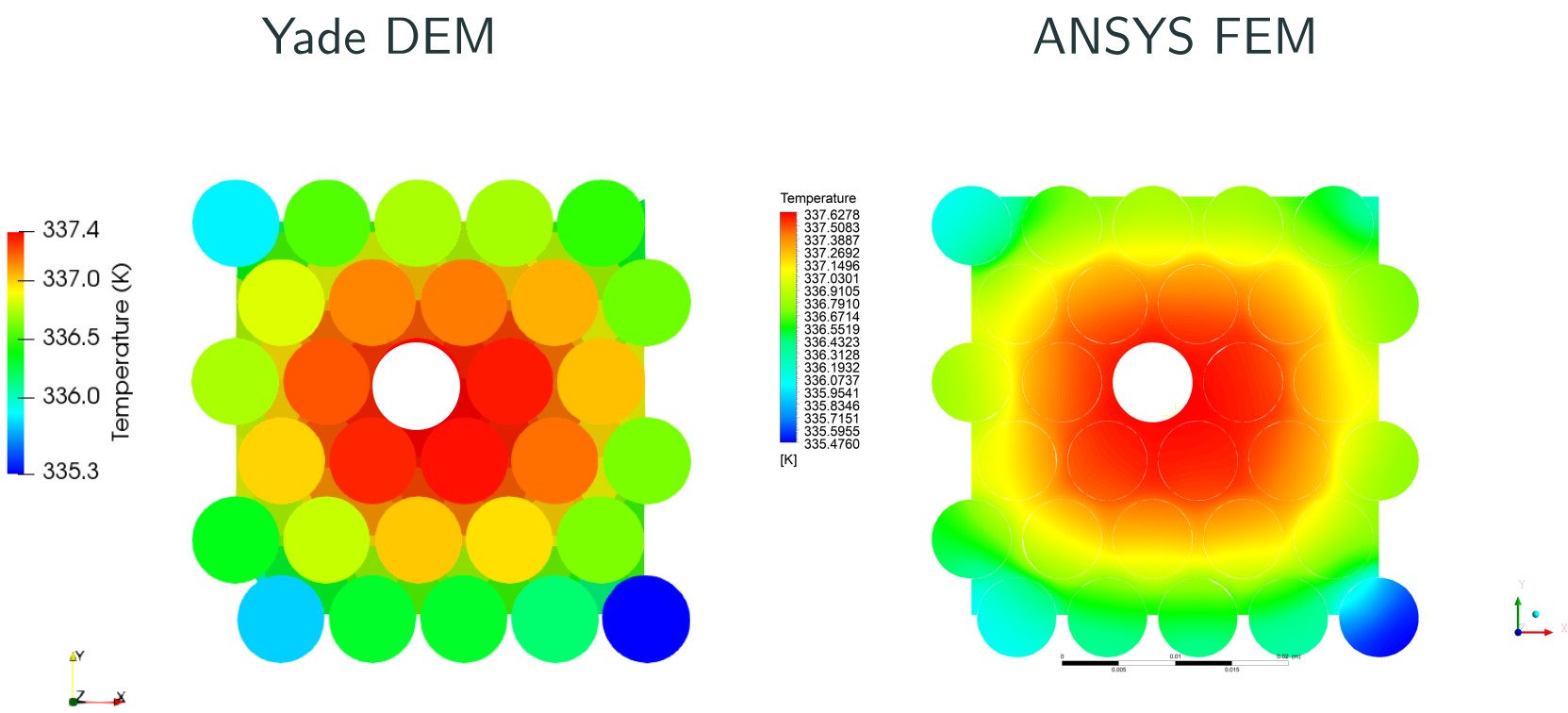


Figure 6: Cross sectional temperature distributions for DEM and FVM in no-flow scenario for t=30 seconds

Numerical validation: Flow condition

Flushing 70°C water through 60°C sphere packing:

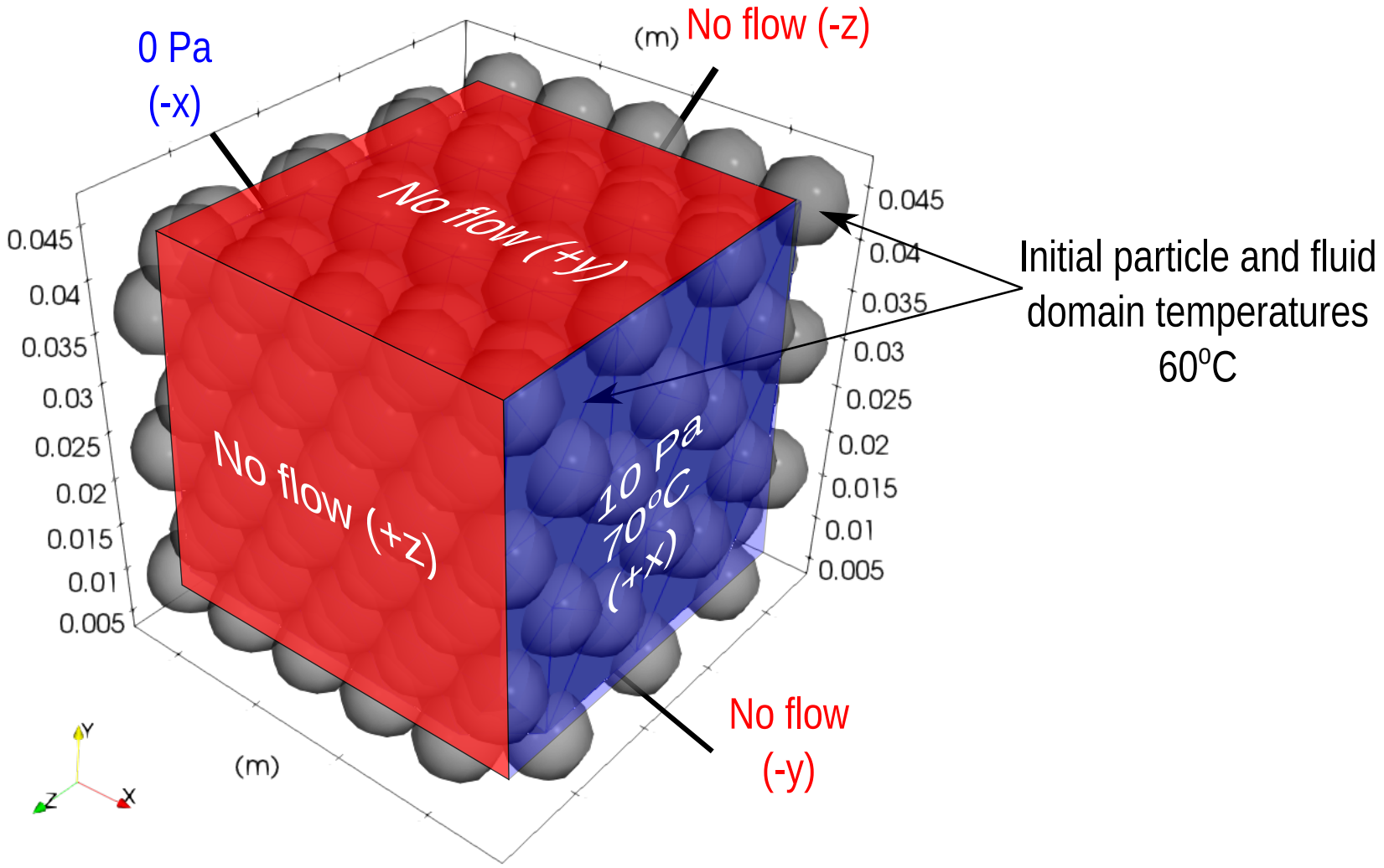


Figure 7: Specimen dimensions and boundary conditions for Yade DEM and ANSYS FEM Flow

Numerical validation: Flow condition

Flushing 70°C water through 60°C sphere packing:

Numerical validation: Flow condition

Yade DEM

ANSYS CFX

Numerical validation: Flow condition

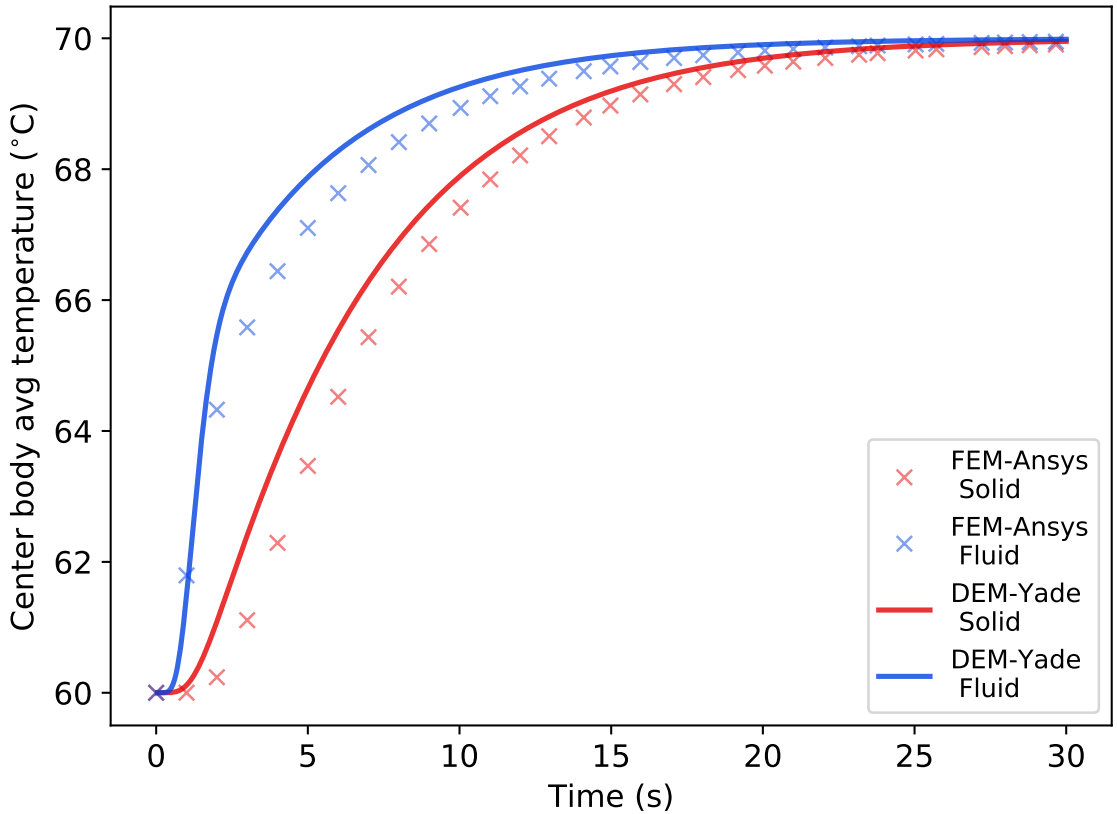
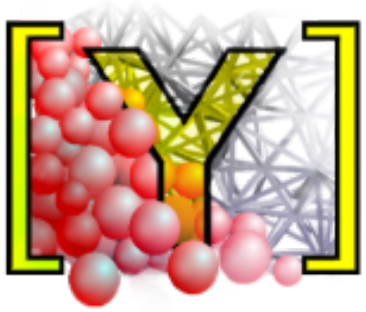


Figure 8: ANSYS FEM hot flushing of cold sphere packing validation.

Numerical validation: computational comparison



vs

ANSYS® CFX®

	No-flow (hrs)	Flow (hrs)	Cells
Yade git-dc2ecaec (10-core)	0.04	0.06	1000
ANSYS CFX v.19.2 (12-core)	3.78	5.38	3.5 million

Experimental validation

Experimental configuration [4]:

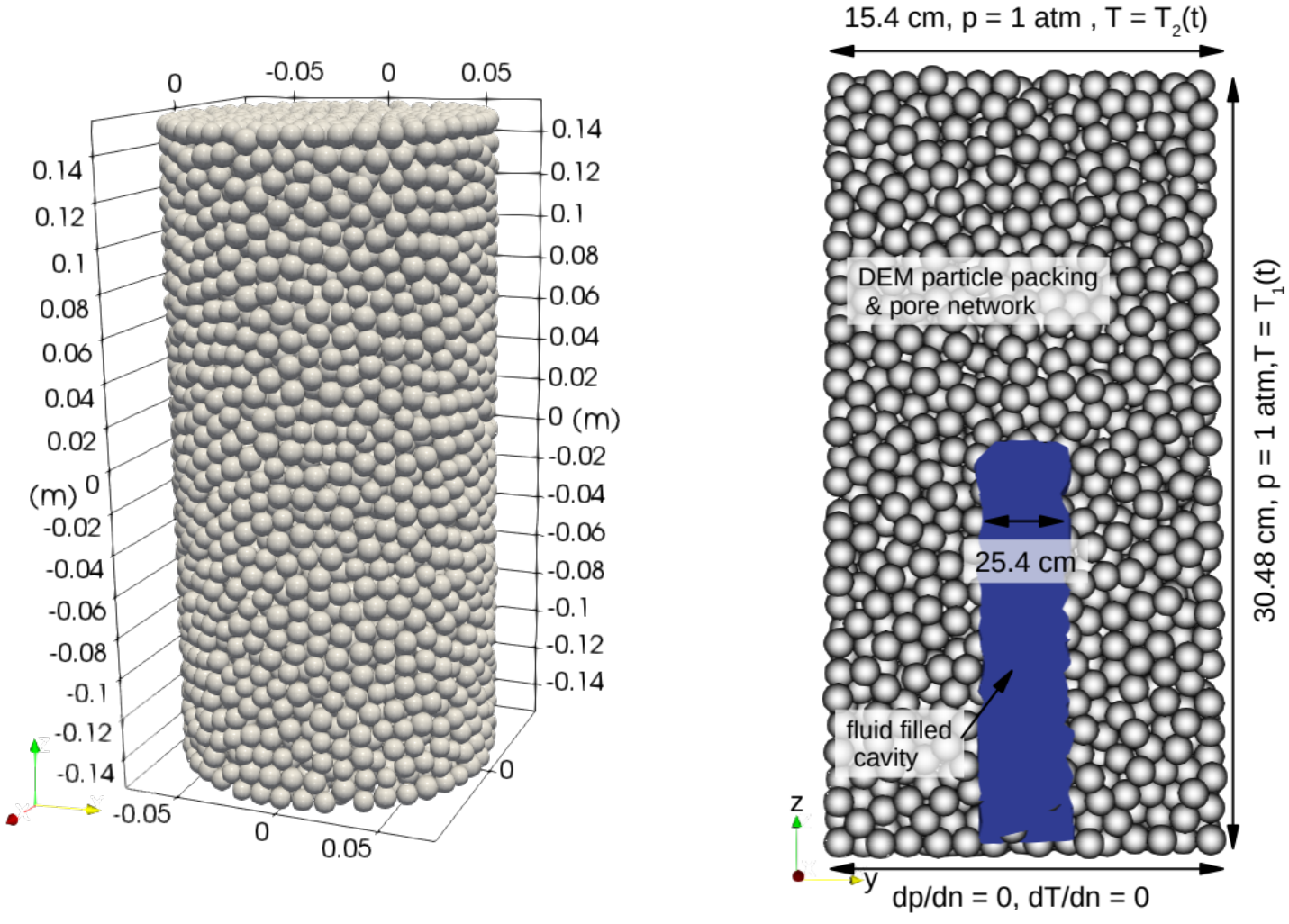


Figure 9: DEM-THM specimen left) Isometric right) split to showing fluid filled inner cavity

Experimental validation

Thermal response:

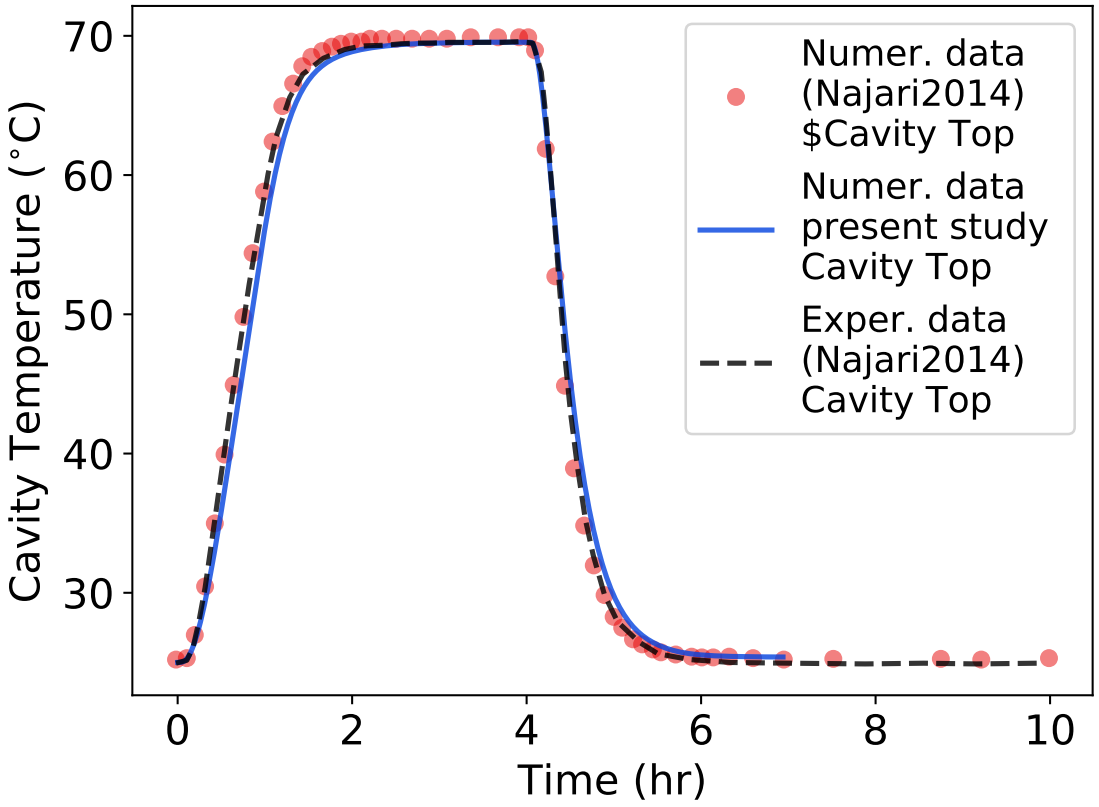


Figure 10: Experimental and numerical cavity temperatures during thermal response test.

Experimental validation

Pressure response:

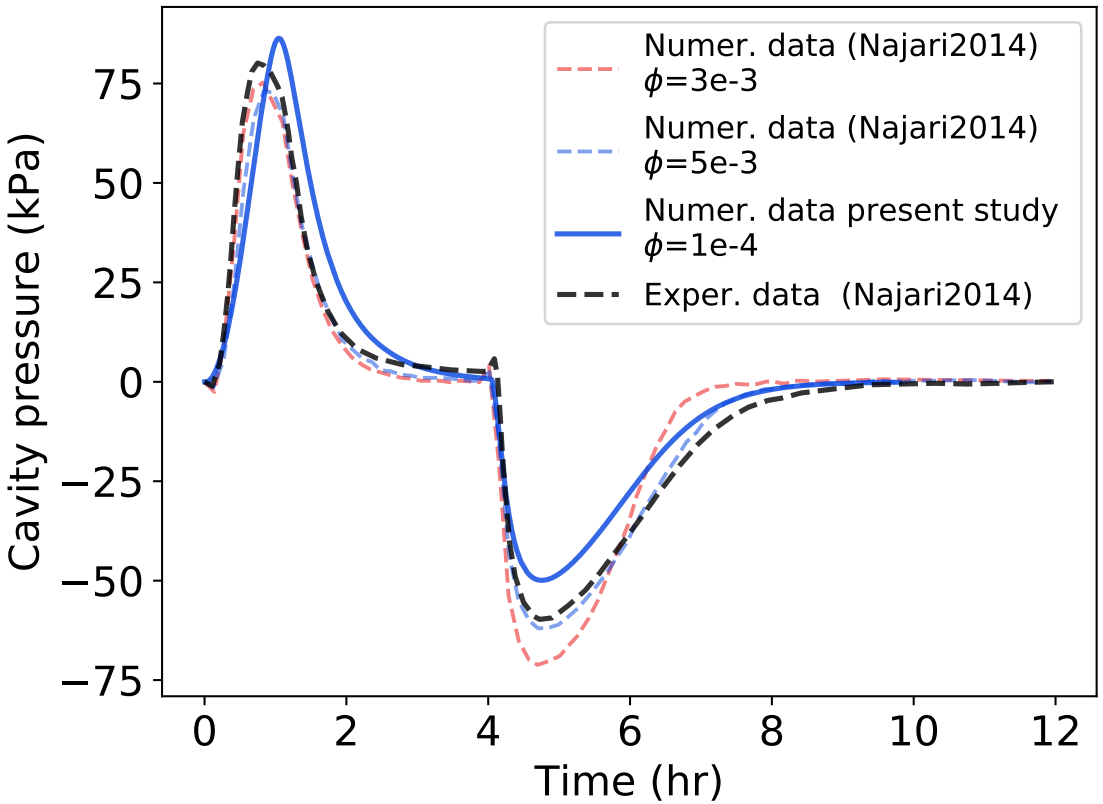


Figure 11: Experimental and numerical cavity pressure curves a) permeability test b) thermal response test

User interface

Adding `ThermalEngine` to Yade's engine list

User simply adds `FlowEngine` and `ThermalEngine` to his/her engine list:

```
O.engines=[
...
FlowEngine(label='flow',thermalEngine=True),
ThermalEngine(label='thermal'),
...
]
```

Setting `ThermalEngine` parameters

Full parameter list available online. Examples below:

```
flow.fluidRho=997 # density
flow.fluidCp=4181.7 # heat capacity
thermal.conduction=True # default true
thermal.advection=True # default: true
thermal.thermoMech=False # default true
thermal.particleAlpha=1e-6 # thermal exp. coeff
thermal.particleK=3 # thermal cond
thermal.particleCp=750 # heat capacity
```

Setting `ThermalEngine` initial and boundary conditions

Initial fluid and particle temperatures:

```
flow.tZero=50 # fluid initial temp
thermal.particleT0=50 # particle initial temp
```

Boundary conditions are available for cuboid packings. Each of the six enclosing walls require boundary condition assignment:

```
# fluid
flow.bndCondIsTemperature=[1,1,0,0,0,0] # constant fluid
↪  temps on x bounds
flow.thermalBndCondValue=[70,60,0,0,0,0] # bound temps
# thermal
thermal.bndCondIsTemperature=[0,0,1,1,0,0] # constant
↪  particle temps on y bounds
thermal.thermalBndCondValue=[0,0,70,60,0,0] # bound temps
```

Data mining in `ThermalEngine`

VTK output for temporal visualization of particle and pore temps accessible by adding the following to the engine list:

```
O.engines=[
...
VTKRecorder(recorders=['spheres','thermal']), # save sphere
↪  positions and temps
PyRunner(command='flow.saveVTK()') # save pore pressures and
↪  temps
...
]
```

Body and pore temperatures are accessible during the simulaton on the command line:

```
bodyTemp = body.state.temp
poreTemp = flow.getPoreTemperature((0,2,1)) # temperature at
↪  coords
```

Conclusions

(1) Developed open sourced thermo-hydro-mechanical framework for geomechanical applications

(2) Verified the code and validated the models experimentally and numerically

(3) Introduced user interface for activating, manipulating, and post processing any Yade THM simulation

Acknowledgements

This work was supported by the Chateaubriand Fellowship of the Office for Science & Technology of the Embassy of France in the United States. Special thanks to Veronica Eliasson and Luc Scholtés for academic support.

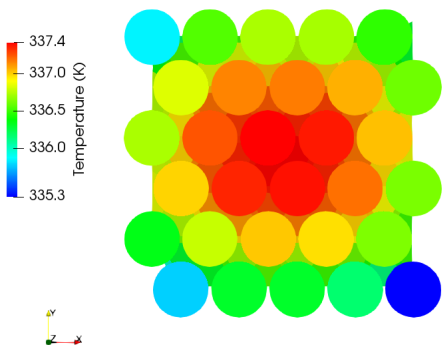
Chateaubriand

Fellowship Program

Science, Technology, Engineering, Math & Health

Questions?

Yade DEM



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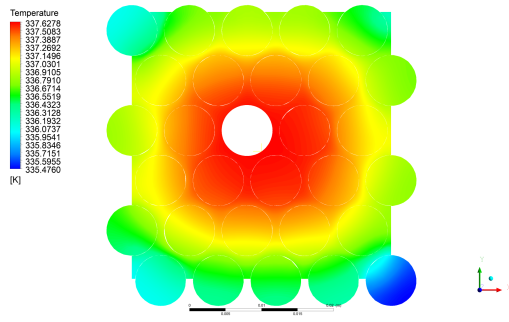

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email: rob.caulk@gmail.com

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References ii

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