# On modeling freezing front propagation in samples of saturated porous medium

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# Motivation - global

- thaw - freeze cycles, climate changes in arctic regions and consequences
- structural changes in constructions
- fabrication of advanced materials
- phase change energy storage
- thaw - freeze cycles, local regions
- seasonal structural changes in constructions

frost patterns on soil surface

frost heave damaging constructions

vegetation patters generated by winter freezing

## Outline of the talk

1. Motivation
2. Phenomena
   - scales
   - layer effects
3. Experiments
   - geometry, measurement
4. Mathematical models
   - balance laws
   - phase transition
5. Computational studies
   - single pore
   - grain curvature vs. phase interface
6. Conclusion and perspectives

## Joint work:

- Faculty of Nuclear Sciences and Physical Engineering (P. Strachota, M. Kolář, M. Narayanan)
- Faculty of Civil Engineering, CTU Prague (M. Sněhota, M. Sobotková, J.F. Kubát)
- Colorado School of Mines (T.H. Illangasekare)
- U.S. Army Engineer Research and Development Center, Vicksburg (A.C. Trautz, M. Farthing)


## Acknowledgement

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- *Complex multiscale and multiphase processes related to freezing and thawing in porous media*, project No. 1225201X000 of the Fund for Future of the Czech Technical University in Prague, 2024
- *Multiphase flow, transport, and structural changes related to water freezing and thawing in the subsurface*, project No. 21-09093S of the Czech Science Foundation

# Phenomenology

List of phenomena and factors of phase transitions in porous media:

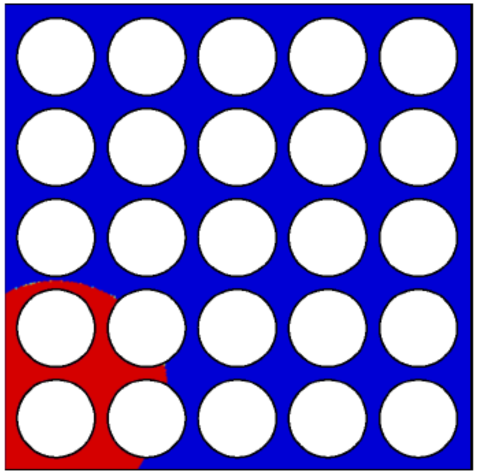
- Heat transfer - controlling mechanism
- Variations in specific volume in solid-liquid transition
- Induced forces causing deformation and motion
- Heterogeneous spatial structure
- Poromechanics
- High-curvature surface phenomena
- Molecular surface contact of phases

Scales:

$10^0 - 10^2$ m

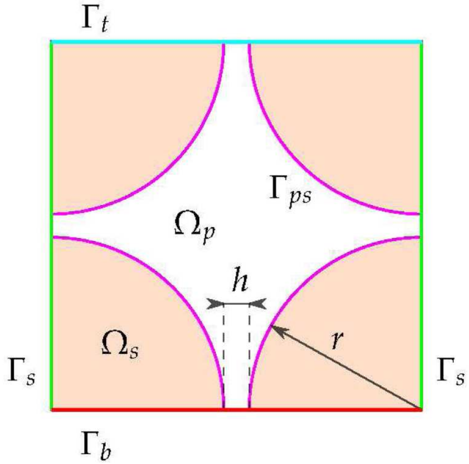
landscape

$10^{-3} - 10^{-5}$ m



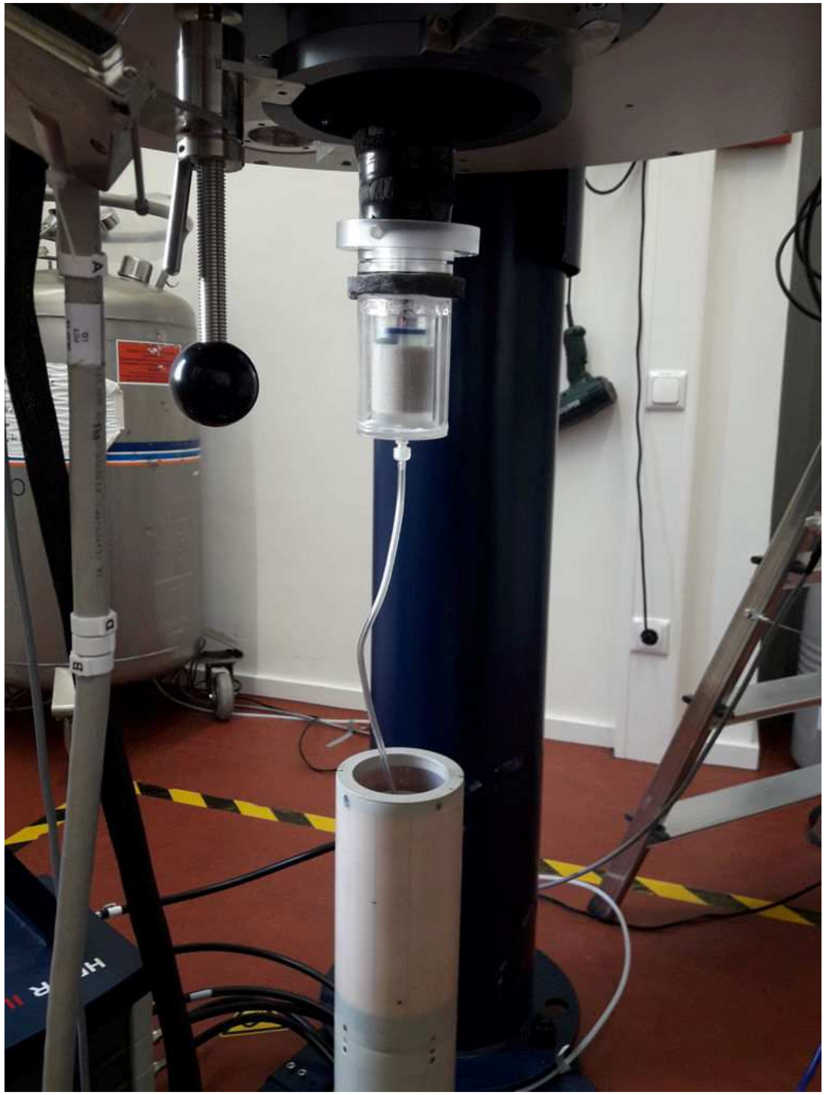
REV with recognized pores

$10^{-6}$ m

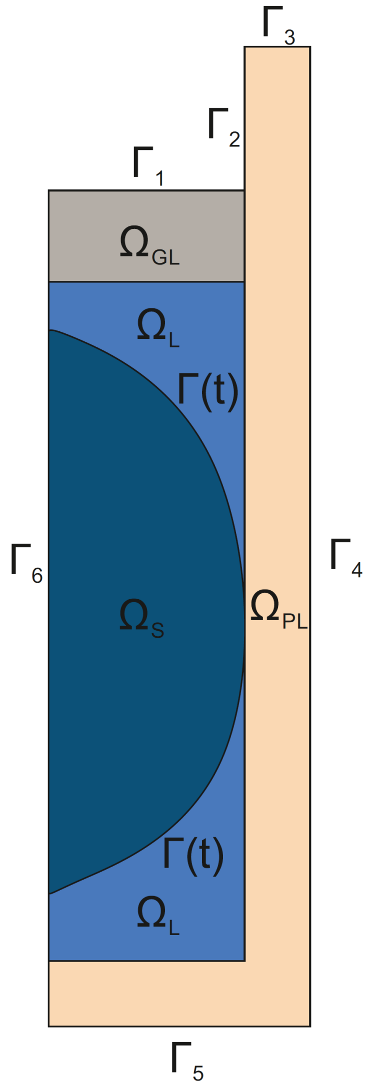



single pore

# Simulation of MRI experiment - setup



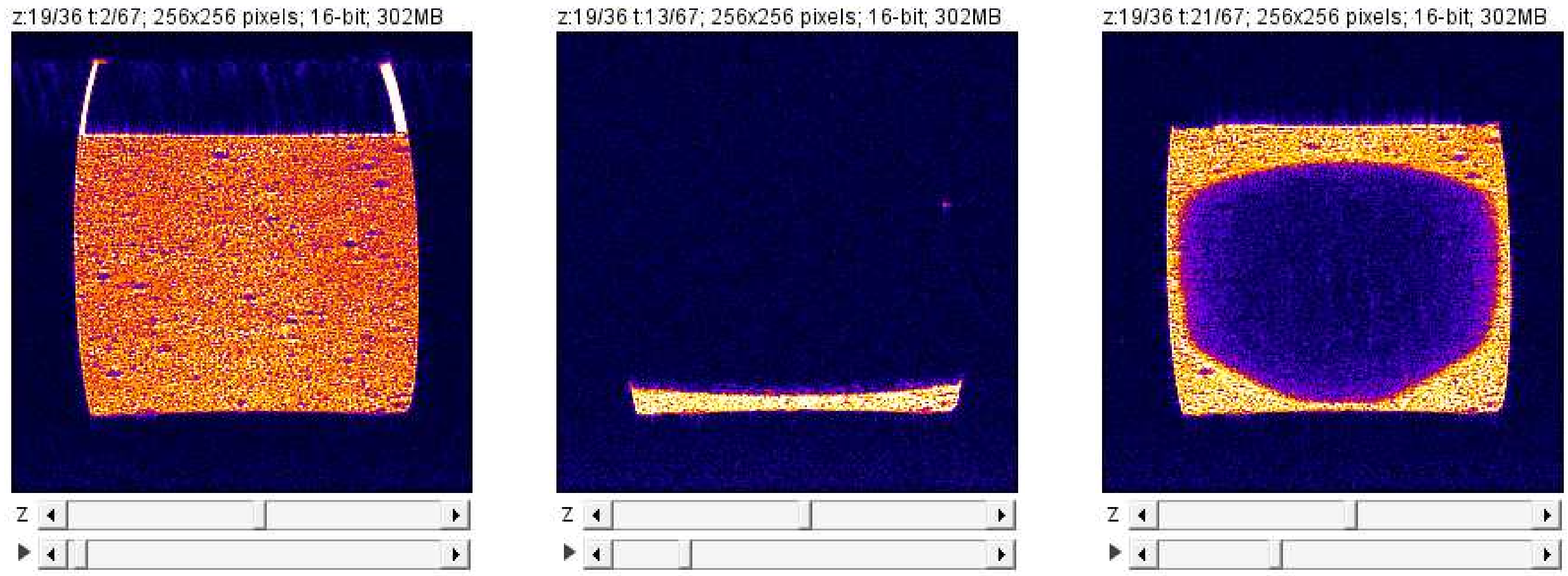
Experimental setup

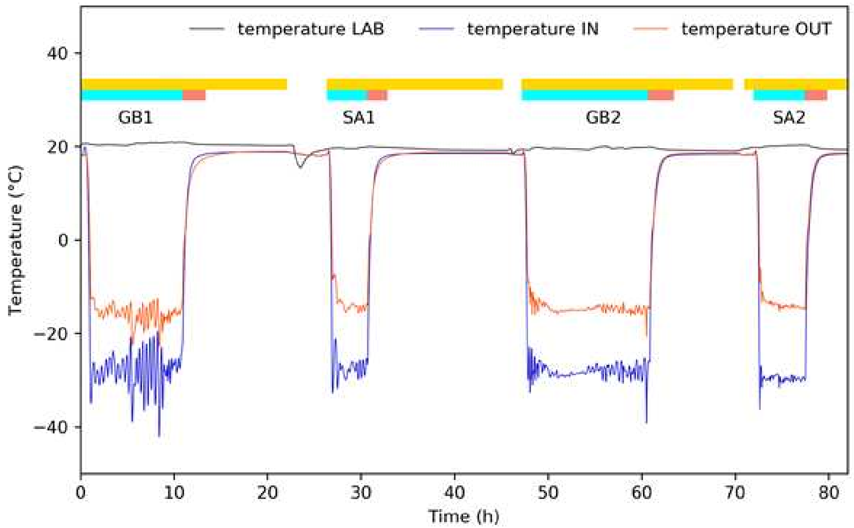



Geometry

*Faculty of Civil Engineering, CTU in Prague*

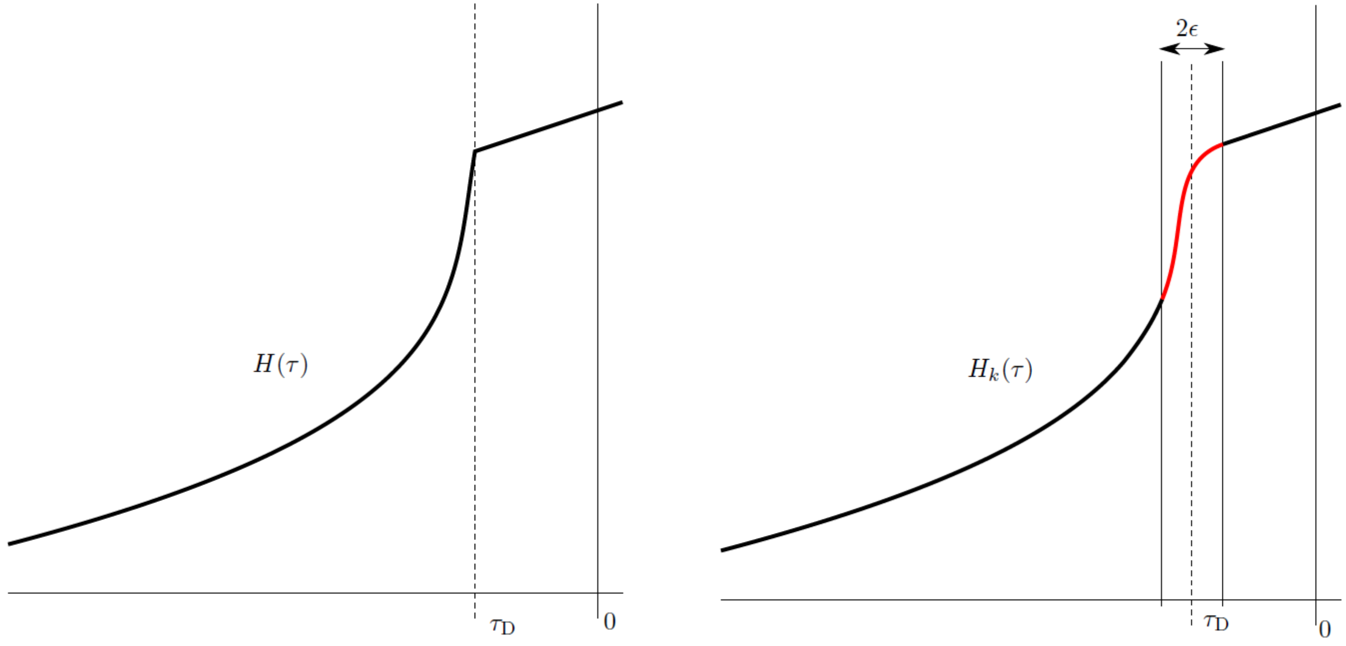
# MRI scans of experiments




Three time snapshots through the center of the container, and temperature control

# Meso-Scale Model - Enthalpy of Saturated Homogenized Medium




Using unfrozen water content with freezing point depression $T_D < 273.15$ K, porosity $\eta$, and $b > 0$

$$\theta(T) = \begin{cases} \eta & \text{for } T \geq T^D \\ \eta \left| \dfrac{T^D - 273.15}{T - 273.15} \right|^b & \text{for } T < T^D \end{cases}$$

enthalpy $H(T)$ is below, and can be regularized ($\epsilon > 0$) to $H_\epsilon(T)$

$$\begin{aligned} H(T) &= \int_{T^{\min}}^{T} \rho_{SS}(T) C_{SS}(T) \mathrm{d}T + \eta L \theta(T) \\ & \rho_{SS}(T) = \eta(T)\rho_{\text{grain}} + (1 - \eta(T)) \left(\theta(T)\rho_{\text{water}} + (1 - \theta(T))\rho_{\text{ice}}\right) \\ & C_{SS}(T) = \eta(T) C_{\text{grain}} + (1 - \eta(T)) \left(\theta C_{\text{water}} + (1 - \theta) C_{\text{ice}}\right) \end{aligned}$$

# Laboratory Meso-Scale Model - enthalpy formulation

Enthalpy formulation of the Stefan problem in the cylindrically symmetric porous medium sample

$$\Omega_{SS} = \Omega_L \cup \Omega_S \cup \Gamma, \text{ with heat conductivity } k_{SS} = k_{\text{grain}}^{\eta} \left( k_{\text{water}}^{\theta} k_{\text{ice}}^{1-\theta} \right)^{1-\eta}$$

$$\partial_t H_\epsilon(T) = \operatorname{div}(k_{SS} \nabla T)$$

and the heat conduction in the container $\Omega_{PL}$ and the cap $\Omega_{GL}$

$$\rho_i C_i \partial_t T = \operatorname{div}(k_i \nabla T)\,, \text{ in } \Omega_i, \; i \in \{PL, GL\}$$

where $\rho_i(x)$ is density, $C_i(x)$ the heat capacity, $k_i(x)$ the heat conductivity of the material $i$.

Continuity of solution and flux at internal boundaries, and boundary conditions

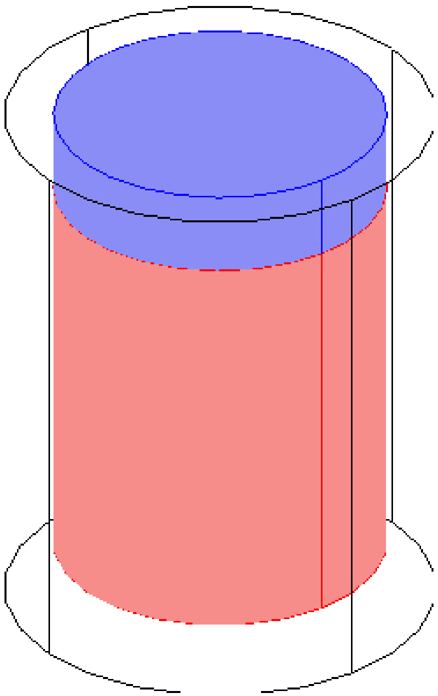
$$-k_{\Omega_j} \frac{\partial T}{\partial n_{\Gamma_i}} = h_{\Gamma_i}(T - T_{\Gamma_i}), \text{ on } \Gamma_i, \quad [i, j] \in B,$$

for $B = \{[1, GL], [2, PL], [3, PL], [4, PL], [5, PL]\}$, $k_{\Omega_j}$ is the heat conductivity of a domain behind the wall $\Gamma_i$, $h_{\Gamma_i}$ is the heat conductivity of the wall $i$ and $T_{\Gamma_i}$ is temperature on the outside of the wall $i$.

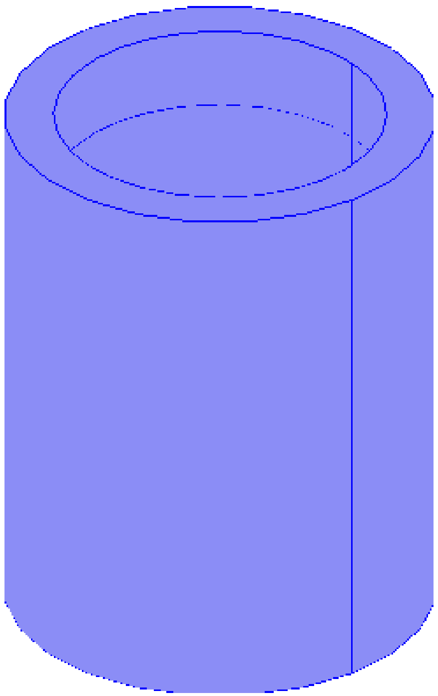
Initial condition

$$T\Big|_{t=t_0} = T_{\text{ini}}$$

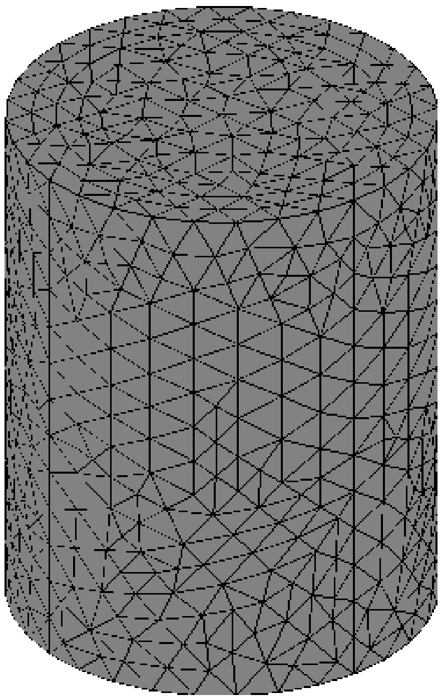
# Simulation setup



Sand and cap



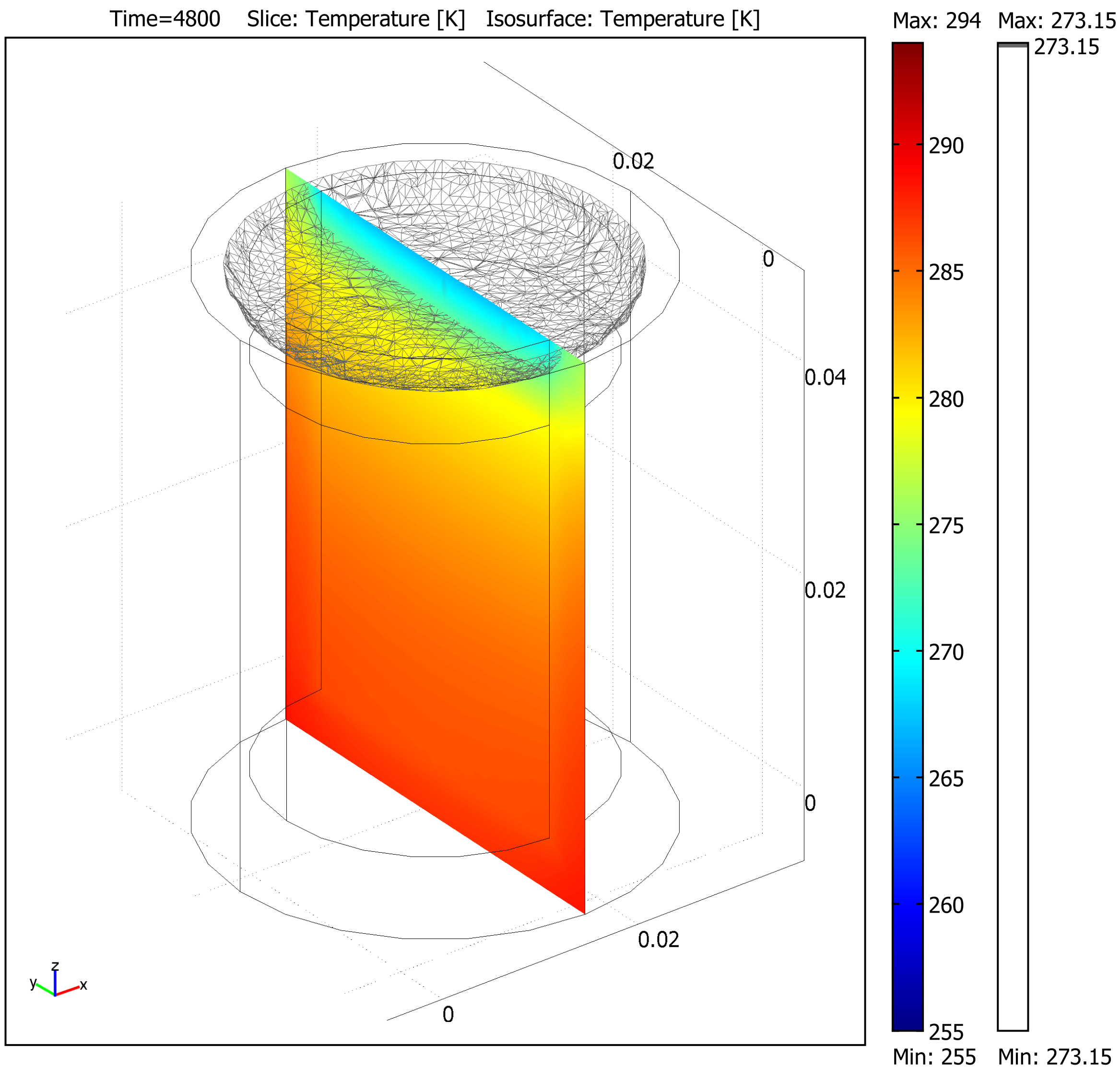
Container



Triangulation

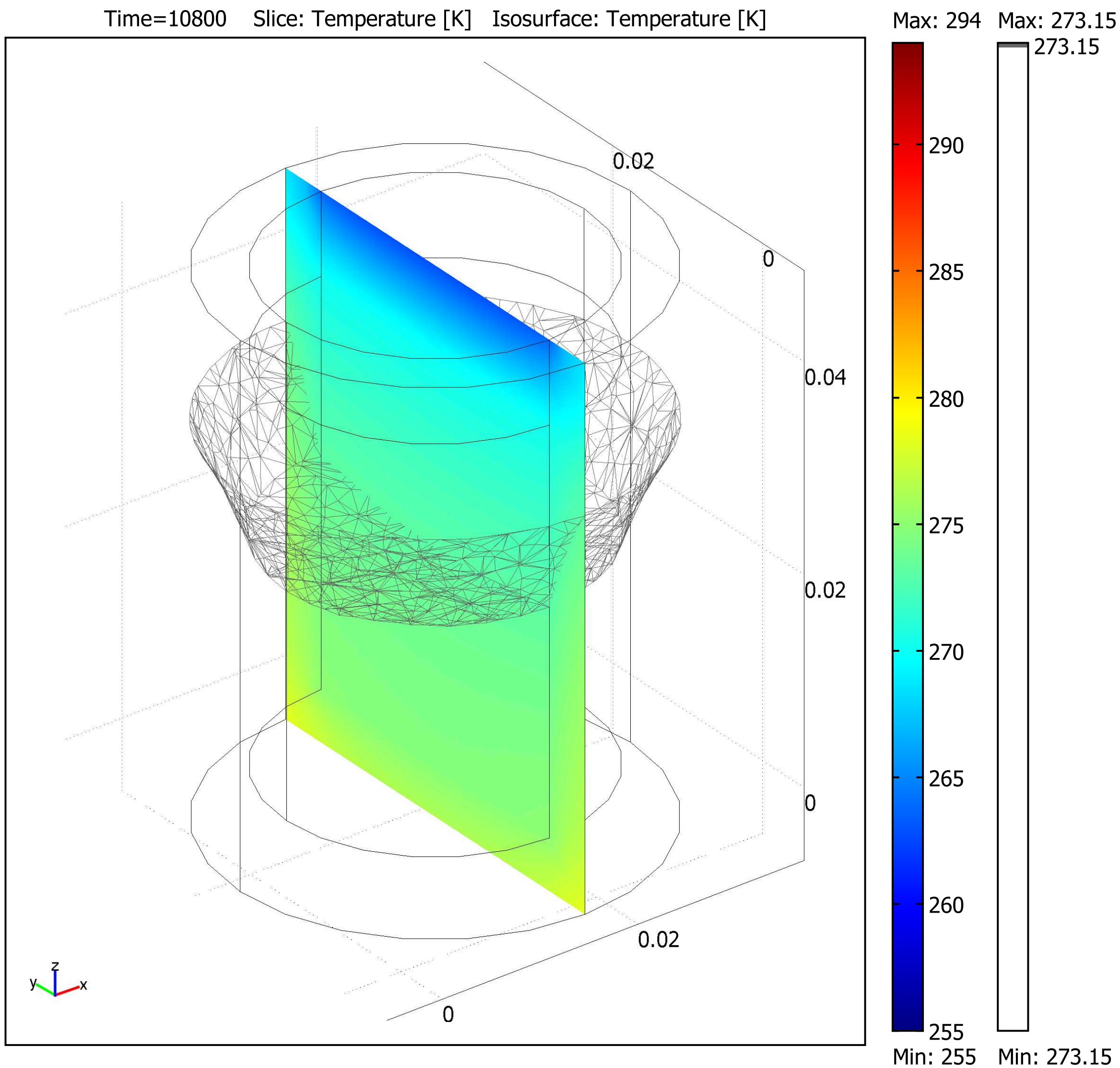
Simulation geometry

# 3D Simulation of MRI experiment with sand



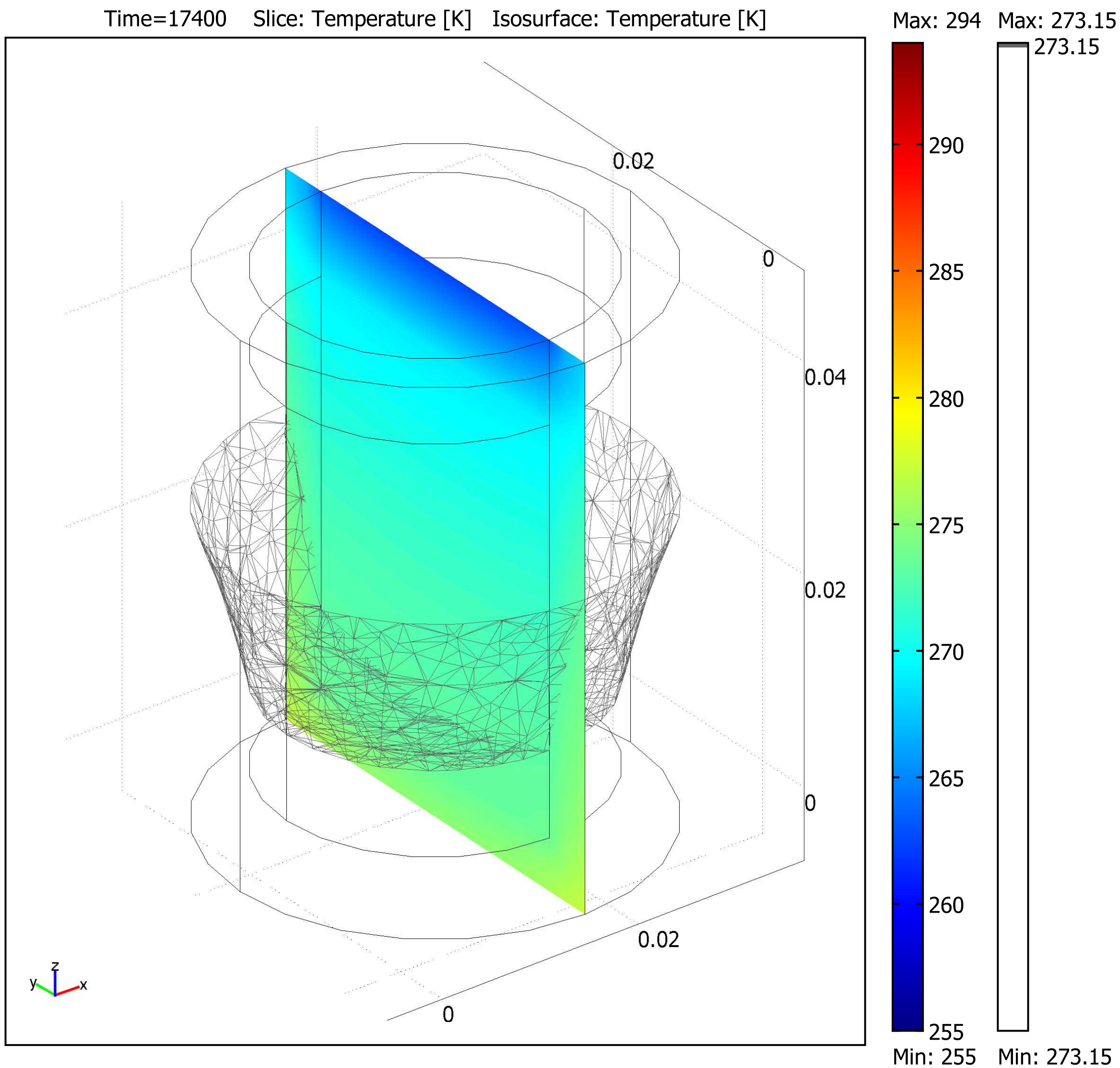

time = 04800 [s]

# 3D Simulation of MRI experiment with sand



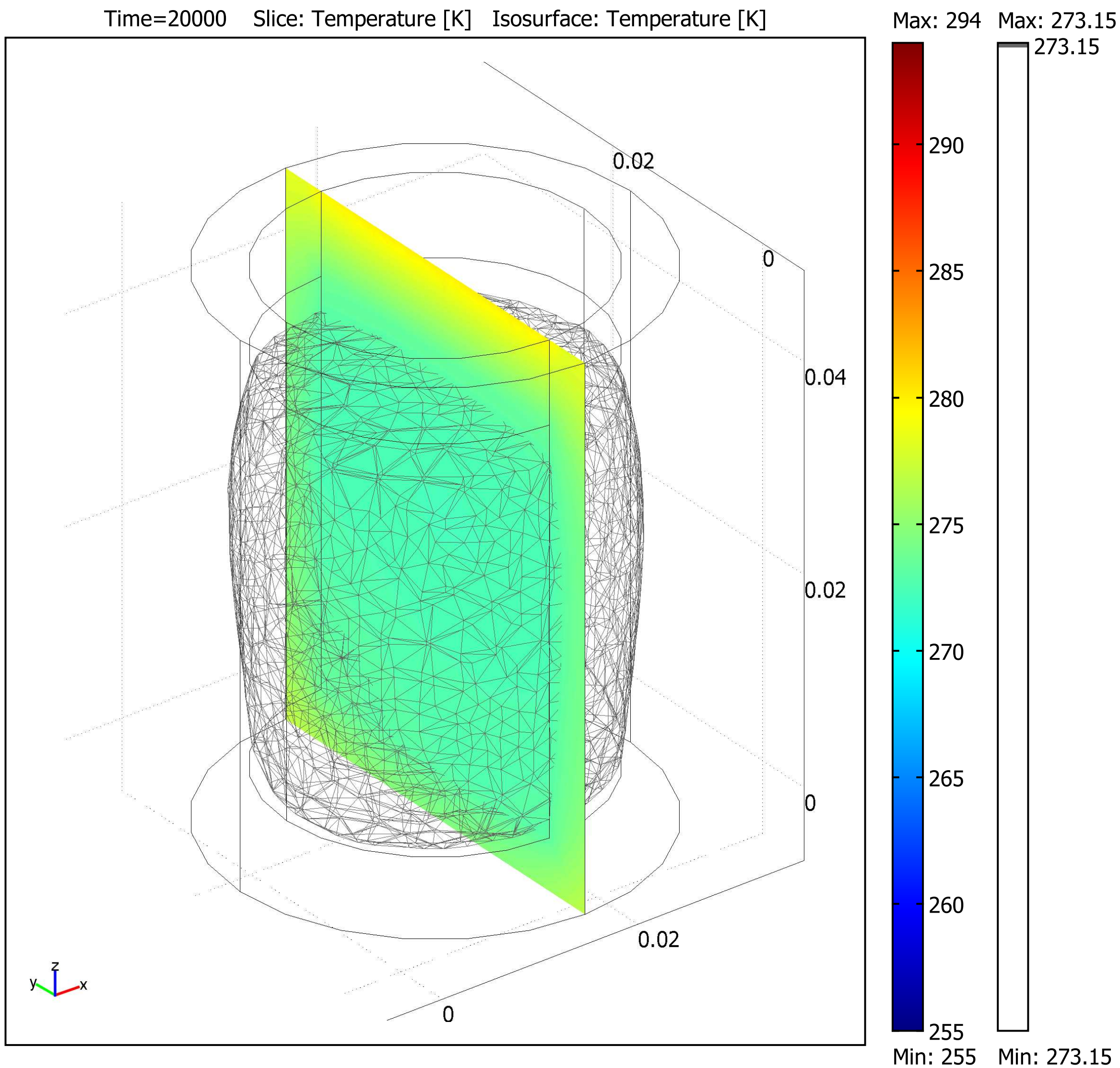

time $= 10800$ [s]

# 3D Simulation of MRI experiment with sand



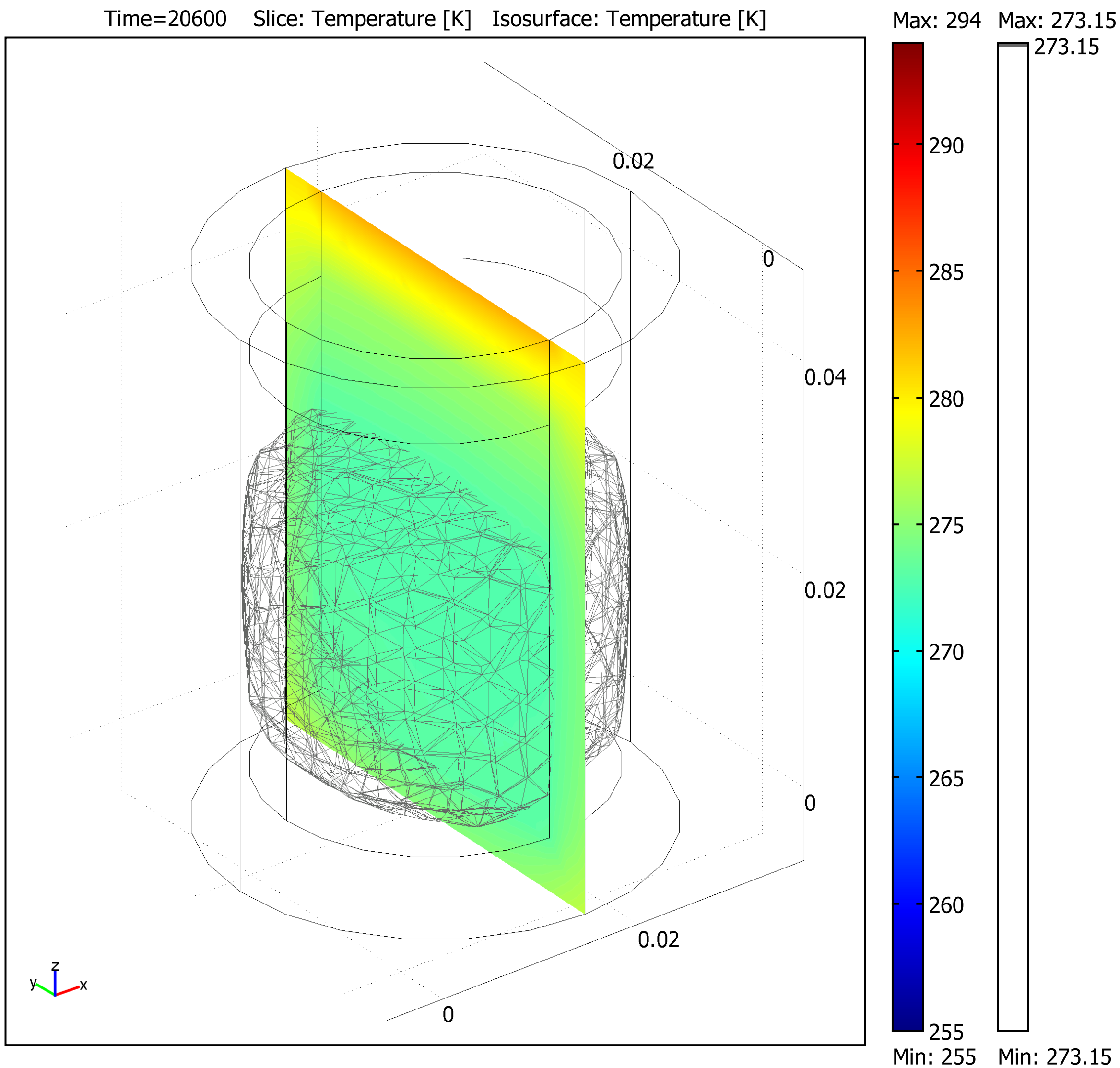

time $= 17400$ [s]

# 3D Simulation of MRI experiment with sand



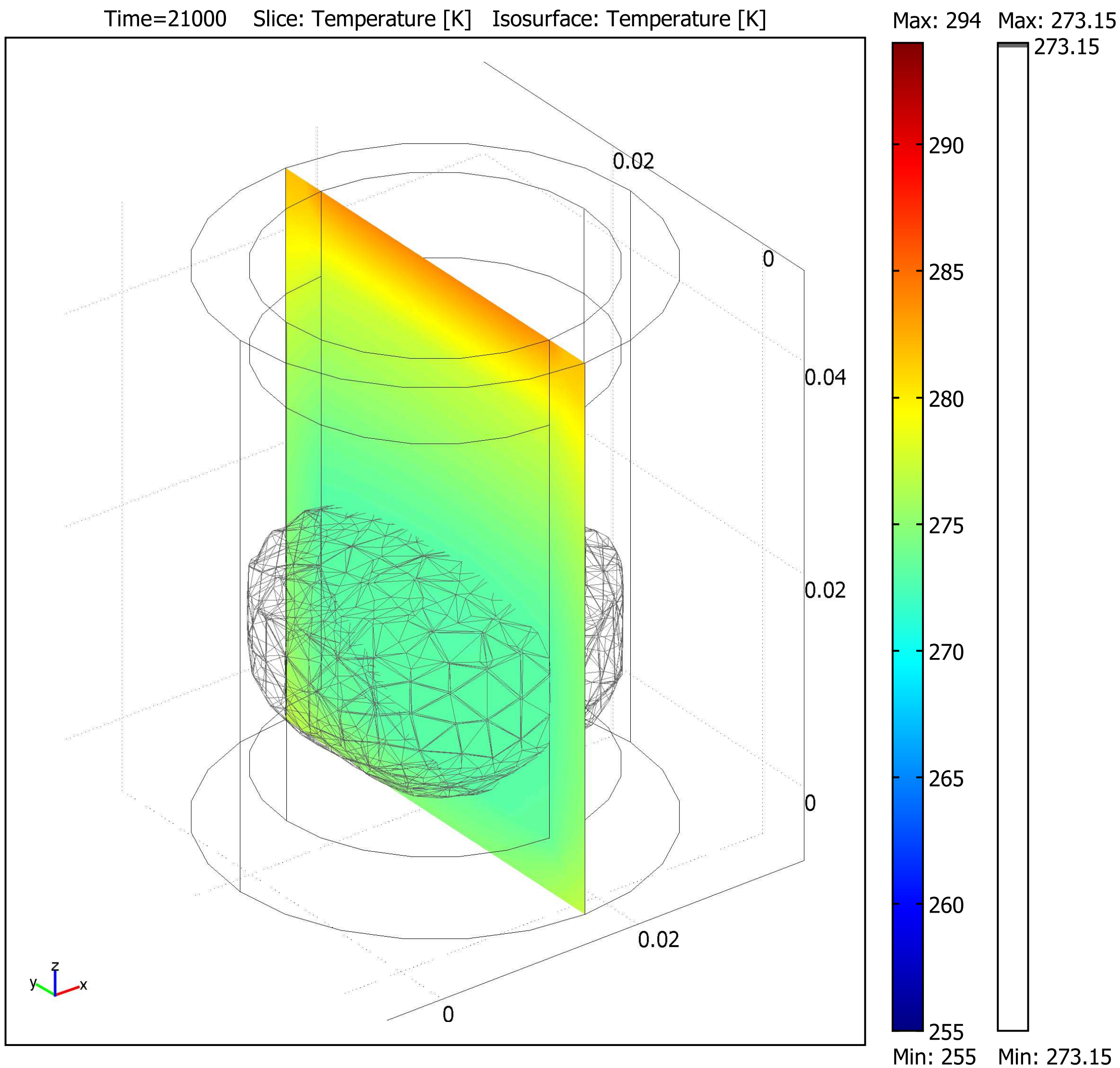

time $= 20000$ $[\mathrm{s}]$

# 3D Simulation of MRI experiment with sand



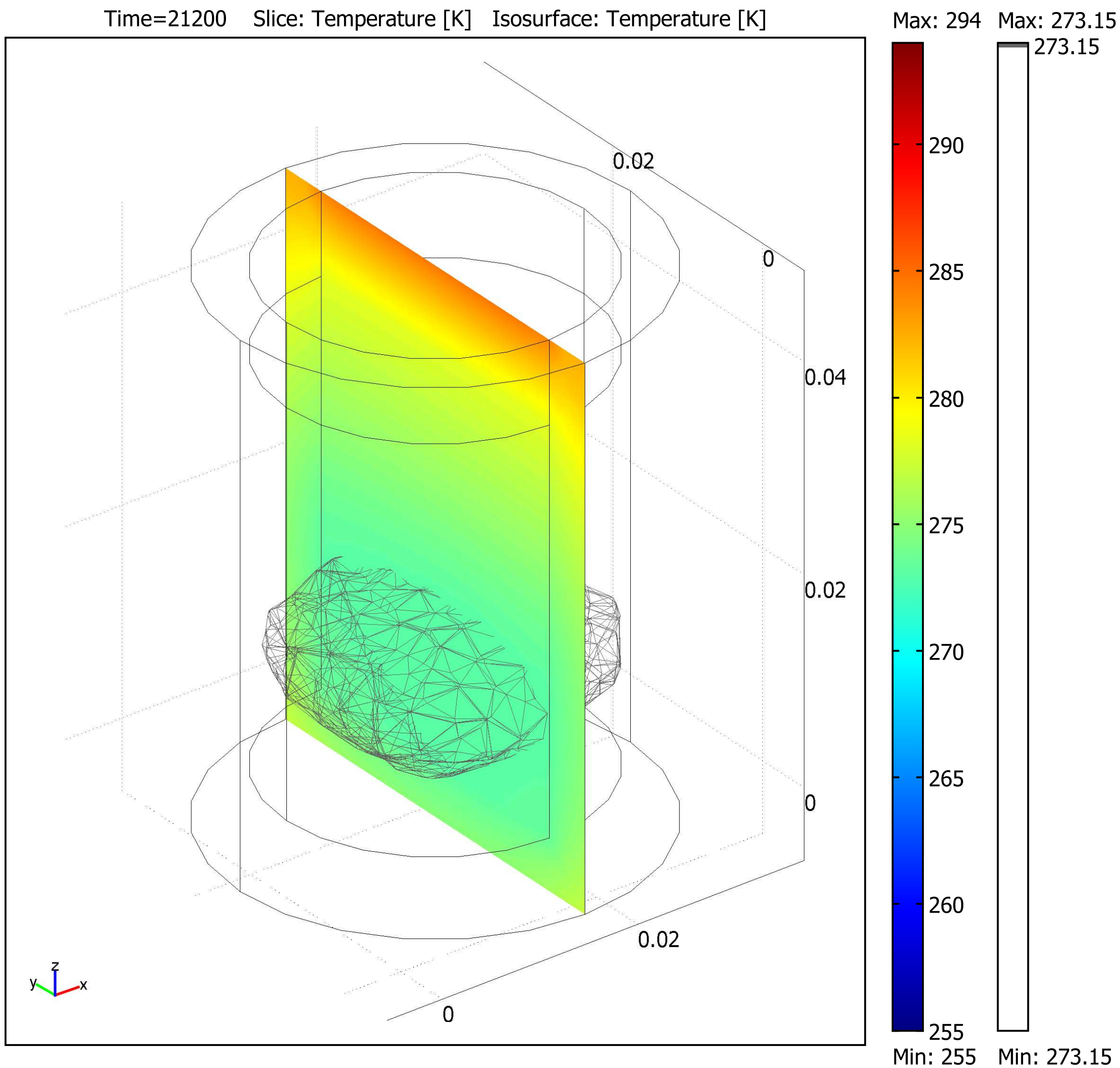

time = 20600 $[\mathrm{s}]$

# 3D Simulation of MRI experiment with sand



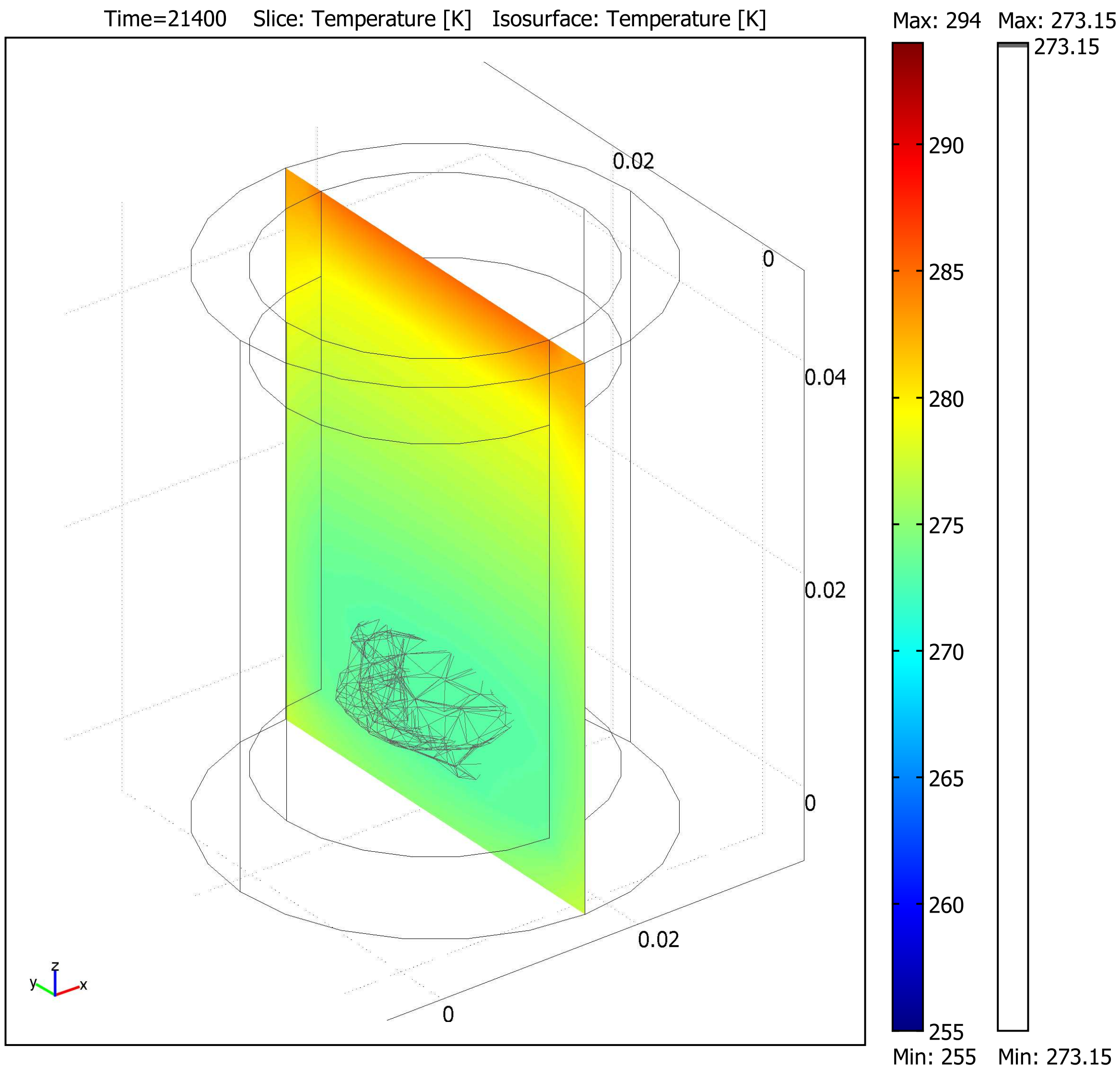

time = 21000 [s]

# 3D Simulation of MRI experiment with sand



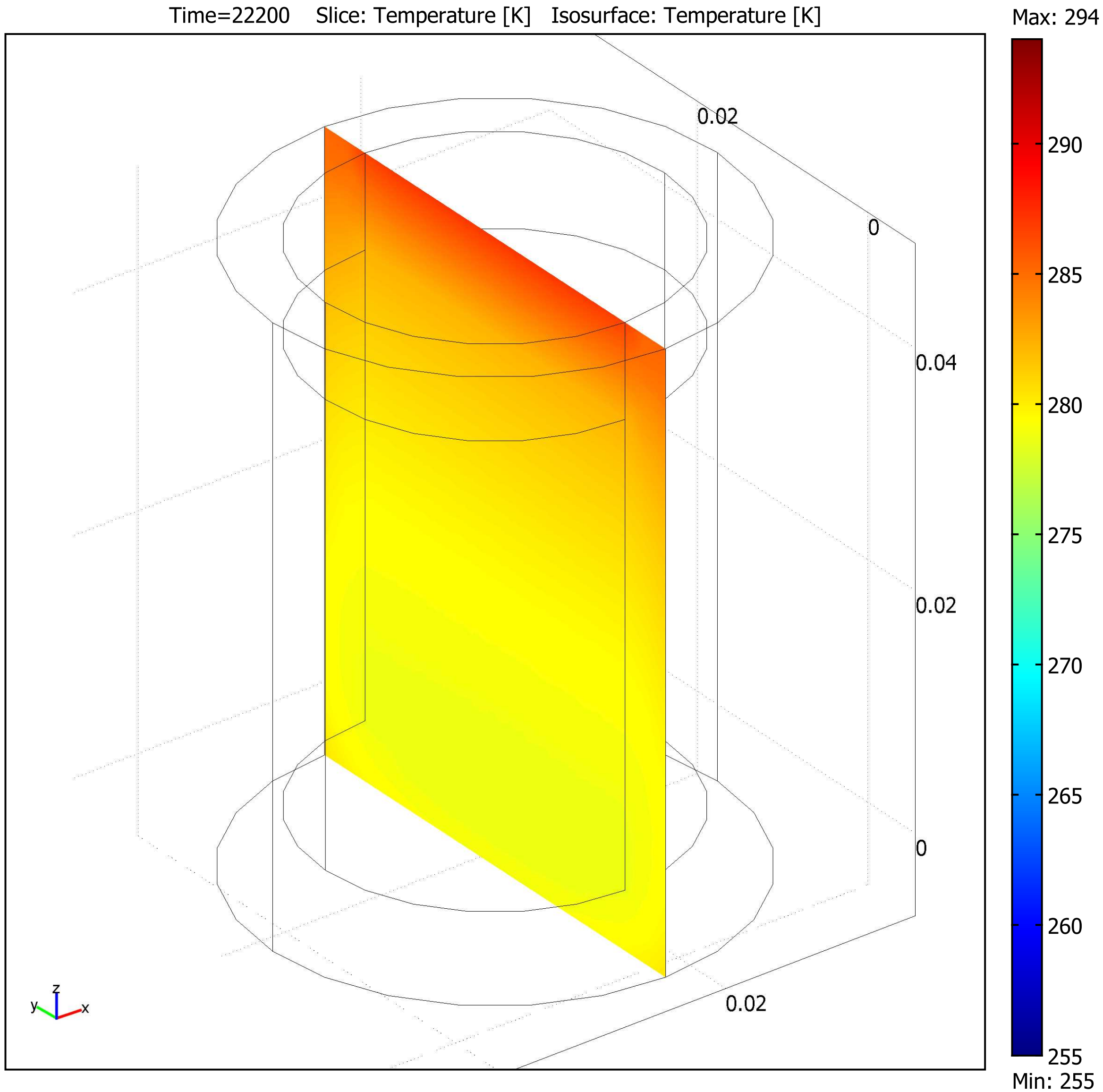

time $= 21200$ [s]

# 3D Simulation of MRI experiment with sand




time = 21400 [s]

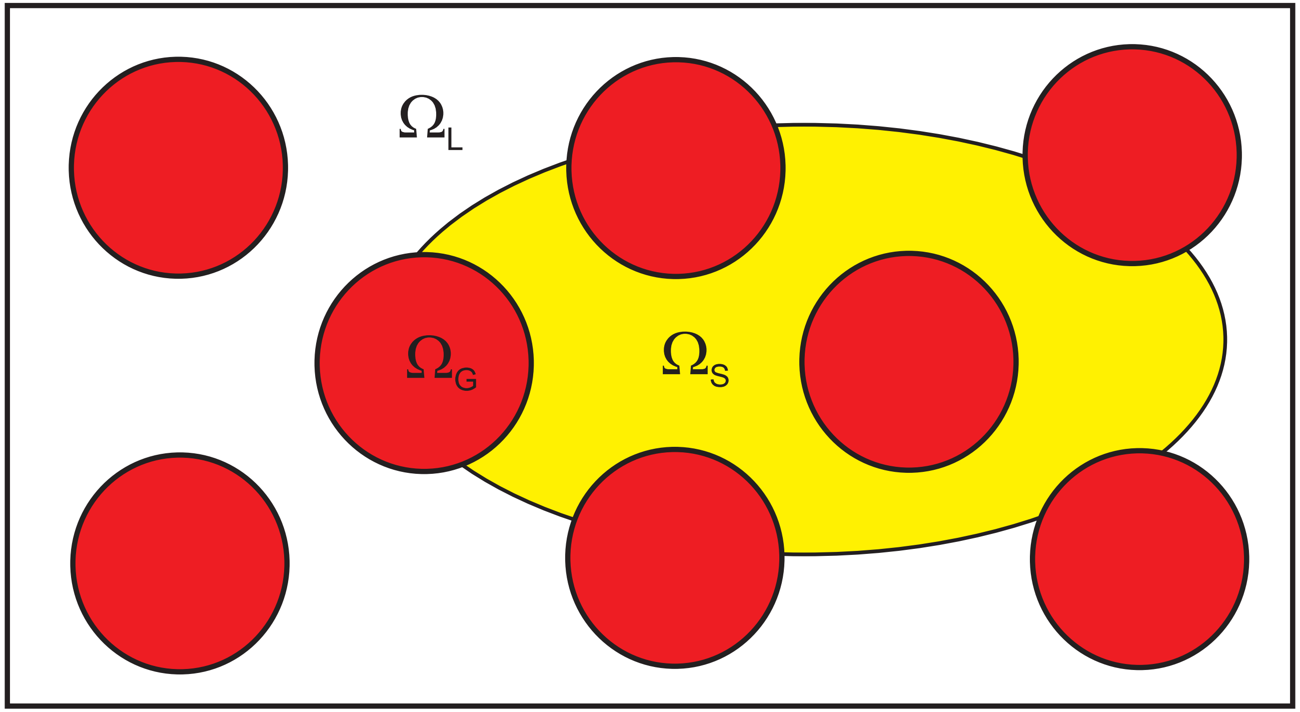
# 3D Simulation of MRI experiment with sand




time = 22200 [s]

# Pore scale model - geometry

Saturated porous medium in pore geometry, ice tracking by phase field




Space domain consists of grains $\Omega_G$ and pores filed by liquid $\Omega_L$ and solidified phase $\Omega_S$

Deformation $\mathbf{u} = \mathbf{u}(t, x)$ in all parts of the domain motivates the use of Lagrangian coordinates

# Phase-Field Micro-Scale Model - notation

Derived for representative microscale on a general pore domain.

- a new function $w = w(t, x)$ with values in $\langle 0, 1 \rangle$
- solid phase $\Omega_S(t) \equiv w(t, x) = 1$
- liquid phase $\Omega_L(t) \equiv w(t, x) = 0$
- phase interface $\Gamma(t) \equiv w(t, x) = \frac{1}{2}$
- function $w$ is obtained from the Allen-Cahn equation

**Reference:**


Žák A. and Beneš M. Micro-Scale Model of Thermomechanics in Solidifying Saturated Porous Media, *Acta Physica Polonica* (2018) 134 (3), 2018, pp. 678–682.

Žák A., Beneš M., Illangasekare T. H. Pore Scale Model of Freezing Inception in Porous Medium, *Comput. Methods Appl. Mech. Engrg.*, Volume 414, 1 September 2023, 116166.

# Phase-Field Micro-Scale Model - equations

Heat balance

$$C(w)\frac{\partial T}{\partial t} = \nabla\cdot(k(w)\nabla T) + L\frac{\partial w}{\partial t} \quad \text{in pores} \qquad C\frac{\partial T}{\partial t} = \nabla\cdot(k\nabla T) \quad \text{in grains}$$

Anisotropic phase field using Finsler geometry (6-fold) in the differential expressions ($T^0$ and $\Phi^0$)

$$\alpha\hat{\xi}\frac{\partial w}{\partial t} = \hat{\xi}\nabla\cdot T^0(\nabla w) + \frac{1}{\hat{\xi}}w(1-w)(w-\frac{1}{2}) + \frac{\Delta s}{\sigma}(T^* - T)\hat{\xi}\Phi^0(\nabla w) \quad \text{in pores}$$

Structural mechanics

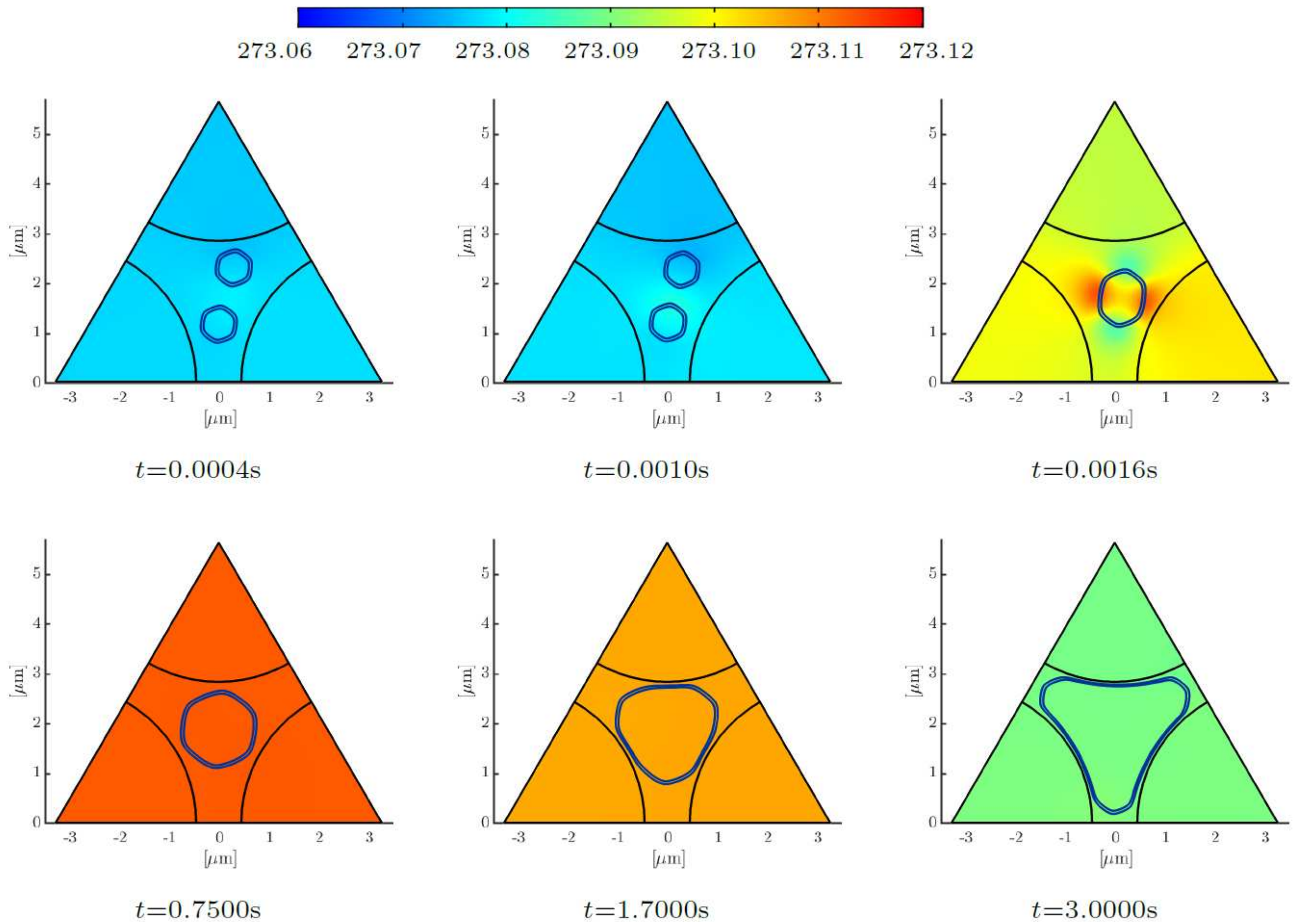
$$\varrho(w)\frac{\partial^2 u_i}{\partial t^2} - \frac{\partial \sigma_{ij}(w)}{\partial x_j} = 0 \quad \text{in all volume}$$

$$\sigma_{ij} = \frac{E_G}{1+\nu_G}\left(\epsilon_{ij}^{el} + \frac{\nu_G}{1-2\nu_G}\epsilon_{kk}^{el}\delta_{ij}\right) \text{ in grains} \qquad \sigma_{ij} = (1-w)\sigma_{ij}^L + w\sigma_{ij}^S + w\bar{\beta}\delta_{ij} \quad \text{in pores}$$

$$\sigma_{ij}^S = \frac{E_S}{1+\nu_S}\left(\epsilon_{ij}^{el} + \frac{\nu_S}{1-2\nu_S}\epsilon_{kk}^{el}\delta_{ij}\right), \quad \text{in pore solid}$$

$$\sigma_{ij}^L = -p(t,x)\delta_{ij} + 2\mu\mathbf{d}_{ij}(t,x), \quad \mathbf{d}_{ij}(t,x) = \frac{1}{2}\left(\frac{\partial \dot{u}_{p,i}}{\partial x_j} + \frac{\partial \dot{u}_{p,j}}{\partial x_i}\right) \text{ in pore liquid}$$

# Computational Studies - coalescence

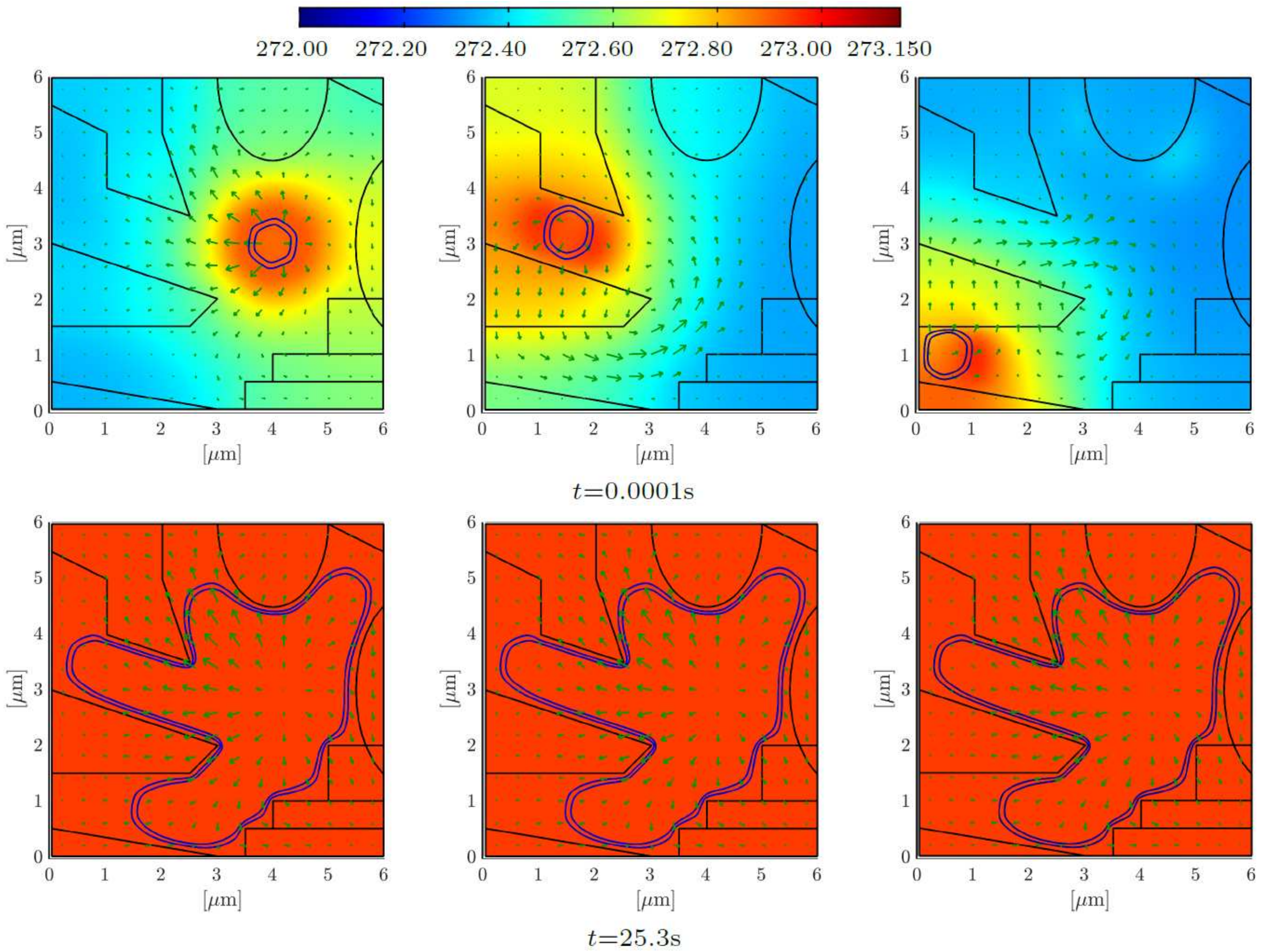



Temperature distribution in color with phase boundaries indicated by double lines

Formation of solid phase, coalescence of two nucleated sites, growth of common pattern and its positioning at pore center

Nucleation sites defined by the initial condition, scale is in $\mu$m

# Computational Studies - independence on nucleation

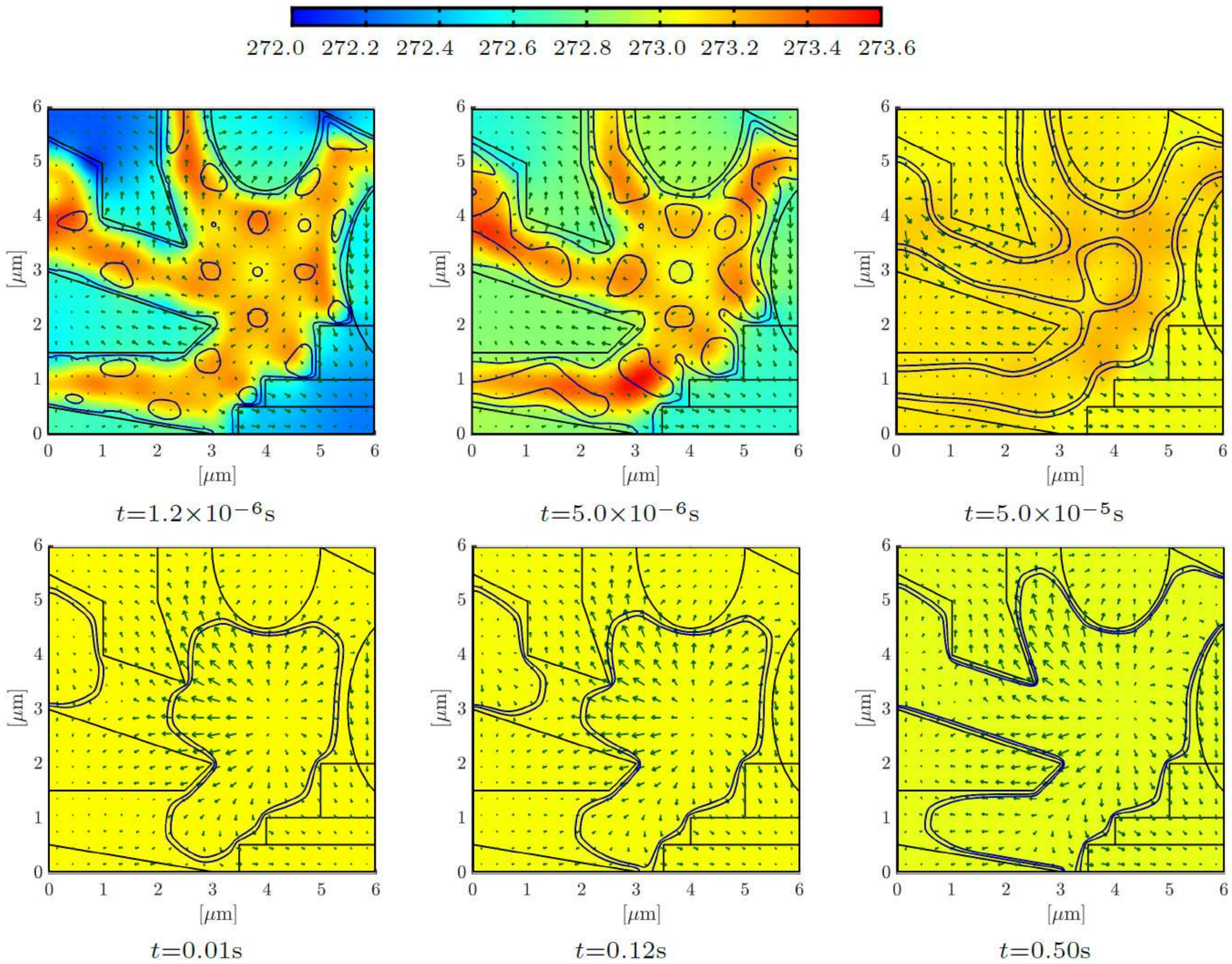



Temperature distribution in color with phase boundaries indicated by double lines

Formation of solid phase starting at three nucleation sites, growth of ice and its repositioning always at pore center

Nucleation sites defined by the initial condition, scale is in $\mu$m

# Computational Studies - homogeneous nucleation




Temperature distribution in color with phase boundaries indicated by double lines

Formation of solid phase started by homogeneous nucleation, growth of ice and its repositioning always at pore center

Nucleation sites defined by the initial condition, scale is in $\mu$m

# Conclusion and Perspectives

**Done**

- density difference in phase transition incorporated
- phase field method tracks the phases, solid-phase anisotropy included
- simplified description of mechanics
- curvature effects at pore scale reconstructed

**Challenges:**

- contact or separation boundary conditions for solid phase
- thin layer transport
- poromechanics
- upscaling
- poromechanics
- unsaturated medium
- infiltration / subsurface flow and heat transport

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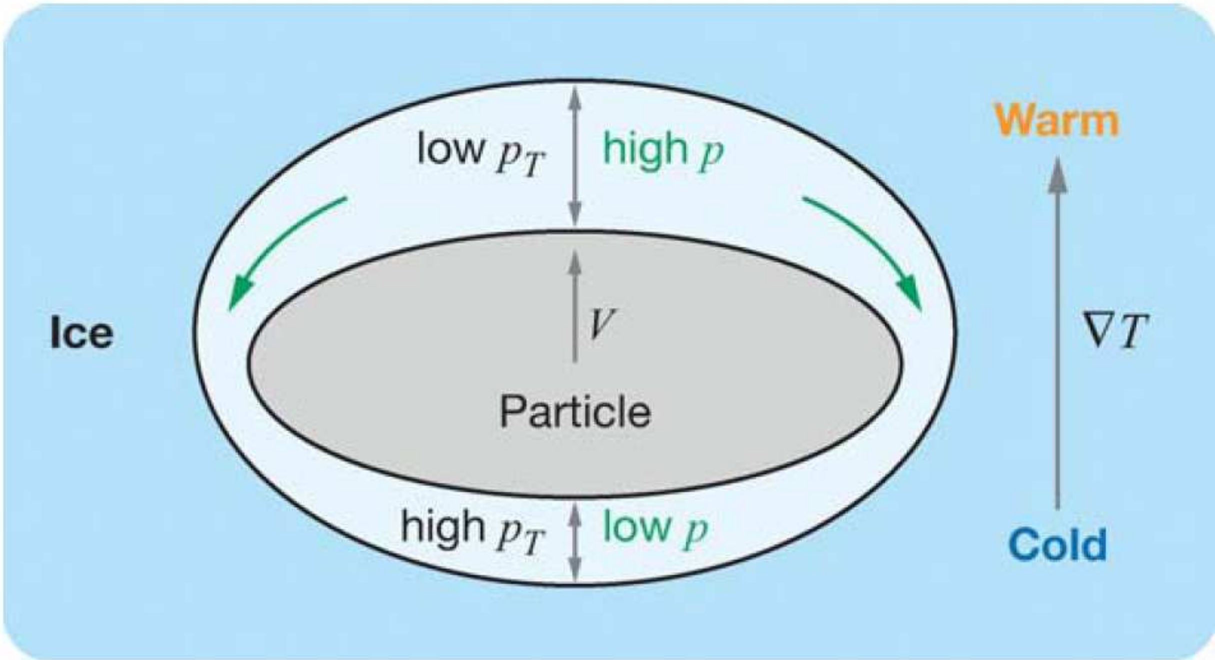
# Premelting, Thin Layers and Porous Media




Schematics of thermal regelation

Force acting on solid object **in the direction** of temperature gradient

$$\mathbf{F}_T = \frac{\varrho_s L}{T^*} \int_{Volume} \nabla T dx$$

Rempel A. W. Microscopic and environmental controls on the spacing and thickness of segregated ice lenses. *Quaternary Research*, 75:316–324, 2011.

# Main idea - Stefan Problem

Clapeyron equation incorporated into the energy balance at microscale

Heat conduction equation:

$$C\frac{\partial T}{\partial t} = \nabla(k\nabla T) \text{ in } \Omega_s \text{ and } \Omega_l$$

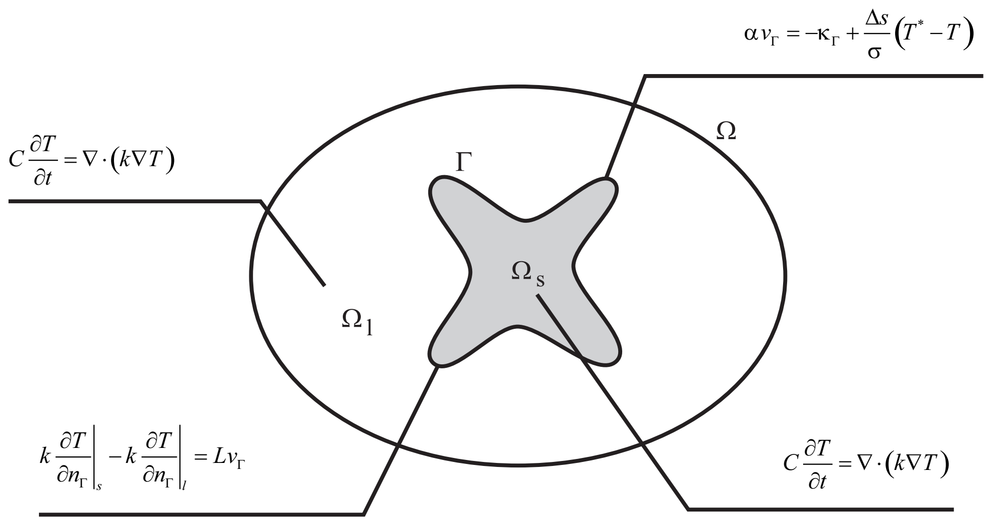
Stefan condition of jump of heat flux:

$$k\frac{\partial T}{\partial n}\,|_s - k\frac{\partial T}{\partial n}\,|_l = L v_\Gamma \text{ on } \Gamma$$

Detection of the phase interface:

$$T - T^* = 0 \text{ on } \Gamma$$

| | |
|---|---|
| $\lambda_s$, $\lambda_l$ | heat conductivity |
| $\Gamma(t)$ | phase boundary |
| $\mathbf{n}_\Gamma$ | normal unit vector to $\Gamma(t)$ pointing out of $\Omega_s$ |
| $v_\Gamma$ | normal velocity of $\Gamma(t)$ |
| $\mathbf{n}_{\partial\Omega}$ | normal unit vector to $\partial\Omega$ pointing out of $\Omega$ |
| $\Omega_L(t)$, $\Omega_S(t)$ | liquid/solid subdomain |
| $T = T(t, x)$ | temperature |
| $L$ | latent heat |
| $T^*$ | freezing point |



# Phase-Field Micro-Scale Model - test functions

Test functions for the weak formulation

- $v_{Tm} \in H^1(\Omega_m)$, $v_{Tp} \in H^1(\Omega_p)$,
- $v_w \in V_w = \{v \in H^1(\Omega_p)| \ v|_{\partial\Omega_p} = 0\}$,
- $\mathbf{v}_{\mathbf{u}m} \in V_{\mathbf{u}m} = \{\mathbf{v} \in H^1(\Omega_m; \mathbb{R}^2)| \ \mathbf{v} \cdot \mathbf{n}_{\partial\Omega_J \cap \bar{\Omega}_m} = 0, \ J = B, L, R\}$,
- $\mathbf{v}_{\mathbf{u}p} \in V_{\mathbf{u}p} = \{\mathbf{v} \in H^1(\Omega_p; \mathbb{R}^2)| \ \mathbf{v} \cdot \mathbf{n}_{\partial\Omega_J \cap \bar{\Omega}_p} = 0, \ J = B, L, R\}$,
- $v_p \in V_p = L^2(\Omega_p)$,

# Phase-Field Micro-Scale Model - weak equalities

Heat - matrix

$$\int_{\Omega_m} \varrho_s c_s \partial_t T v_{T_m} + k_s \nabla T \cdot \nabla v_{T_m} dx + \int_{\partial\Omega} \mathbf{q}_{out} v_{T_m} dS$$
$$+ \int_{\Gamma_+} (wk_i + (1-w)k_w) \nabla T \cdot \mathbf{n}_+ v_{T_m} dS = 0,$$

Heat - pores

$$\int_{\Omega_p} (w\varrho_i c_i + (1-w)\varrho_w c_w) \partial_t T v_{T_p} + (wk_i + (1-w)k_w) \nabla T \cdot \nabla v_{T_p} dx$$
$$- \int_{\Omega_p} \varrho_i l_m \partial_t w v_{T_p} dx + \int_{\partial\Omega} \mathbf{q}_{out} v_{T_p} dS - \int_{\Gamma_+} k_p \nabla T \cdot \mathbf{n}_+ v_{T_p} dS = 0,$$

Phase - pores

$$\int_{\Omega_p} \alpha\xi^2 \partial_t w v_w + \gamma\xi^2 T^0(\nabla w) \cdot \nabla v_w + f_0(w) v_w + \xi^2 \Phi^0(\nabla w) \frac{\varrho_i l_m}{T_M}(T_M - T) v_w dx = 0,$$

Force - matrix

$$\int_{\Omega_m} \varrho_m \frac{\partial^2 \mathbf{u}_m}{\partial t^2} \cdot \mathbf{v}_m + \sigma_m : \nabla \mathbf{v}_m dx + \int_{\Gamma_m} \sigma_p \mathbf{n}_+ \cdot \mathbf{v}_m dS = 0,$$

Force - pores

$$\int_{\Omega_p} (w\varrho_i + (1-w)\varrho_w) \frac{\partial^2 \mathbf{u}_p}{\partial t^2} \cdot \mathbf{v}_p + \sigma_p : \nabla \mathbf{v}_p) dx - \int_{\Gamma_m} \sigma_m \mathbf{n}_+ \cdot \mathbf{v}_p dS = 0,$$

Mass - pores

$$\int_{\Omega_p} (1-w) \left( \frac{p}{\varrho_w E_w} v_p + \nabla \cdot \mathbf{u}_p \cdot v_p \right) dx = 0.$$

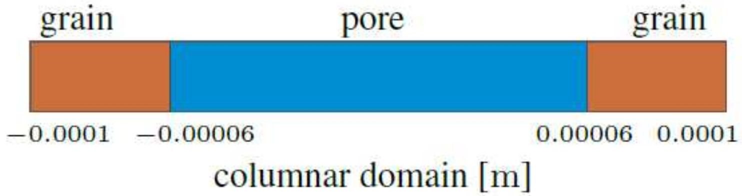
# Phase-Field Micro-Scale Model - Galerkin FEM

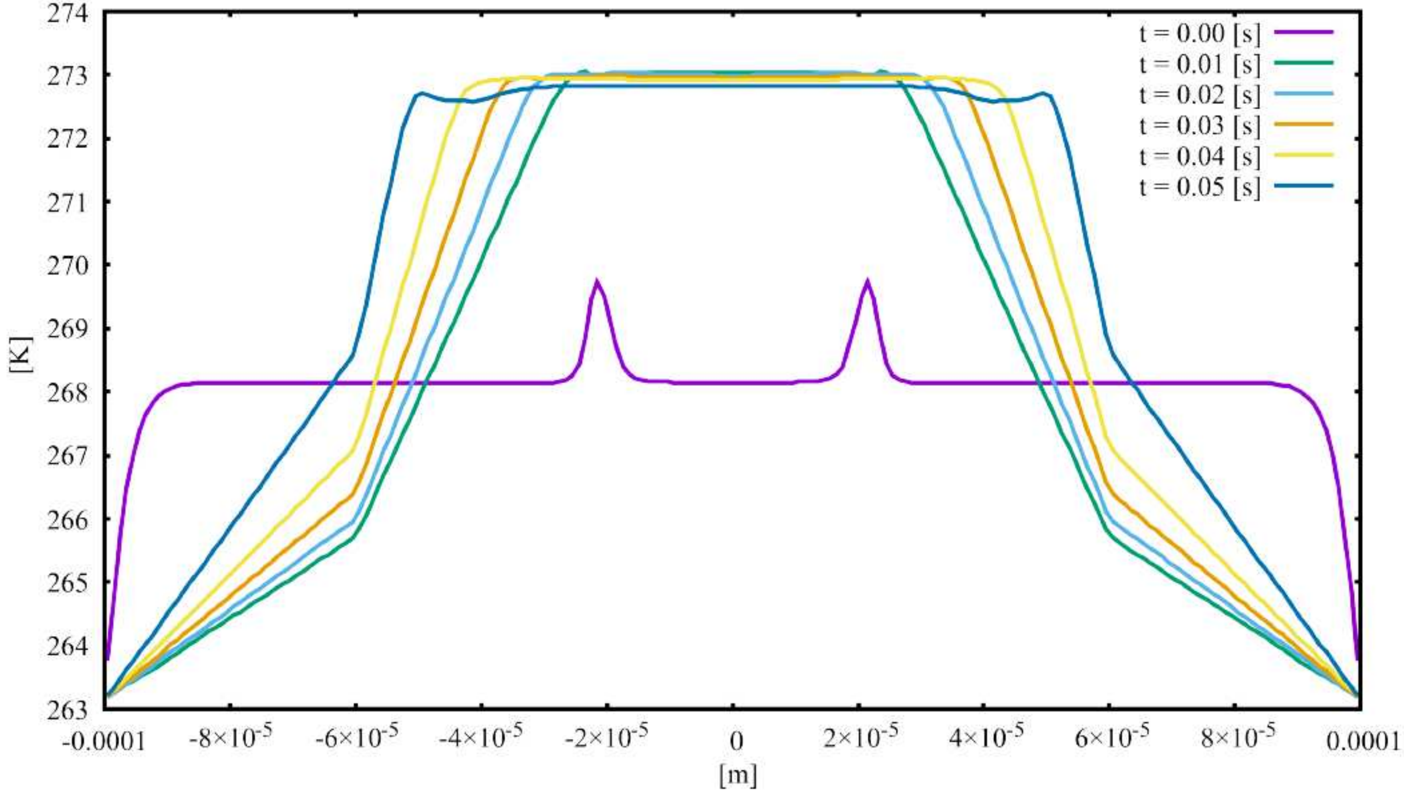
Numerical solution:

- $\Omega$ divided into triangular system $\mathcal{T}_p$ on $\Omega_p$ and $\mathcal{T}_m$ on $\Omega_m$
- quadratic Lagrange elements for FEM
- Faedo-Galerkin approximation applied
- semi-discrete scheme consisting of ordinary differential equations is solved by the generalized $\alpha$-method which is implicit and second-order accurate

J. Chung and G. M. Hulbert. A time integration algorithm for structural dynamics with improved numerical dissipation: The generalized-$\alpha$ method. *Journal of Applied Mechanics*, 60(2):371–375, 1993.

# Computational Studies - columnar growth



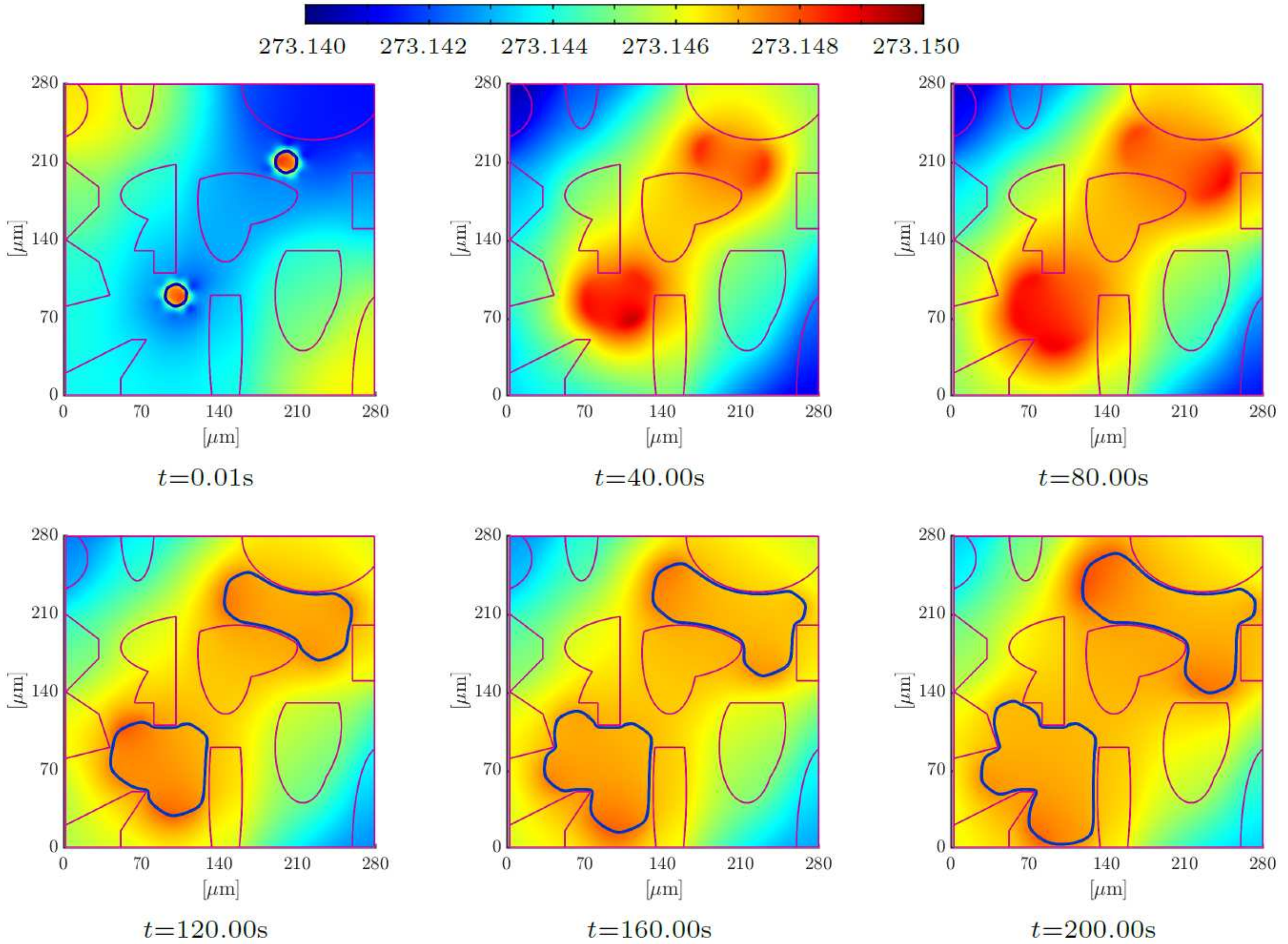




Temperature evolution along 1D column generated by the phase-field model

Formation of solid phase, release of latent heat, growth of ice zone at pore center

Nucleation site defined by the initial condition, scale is in $\mu$m

# Computational Studies - growth in pores - temperature

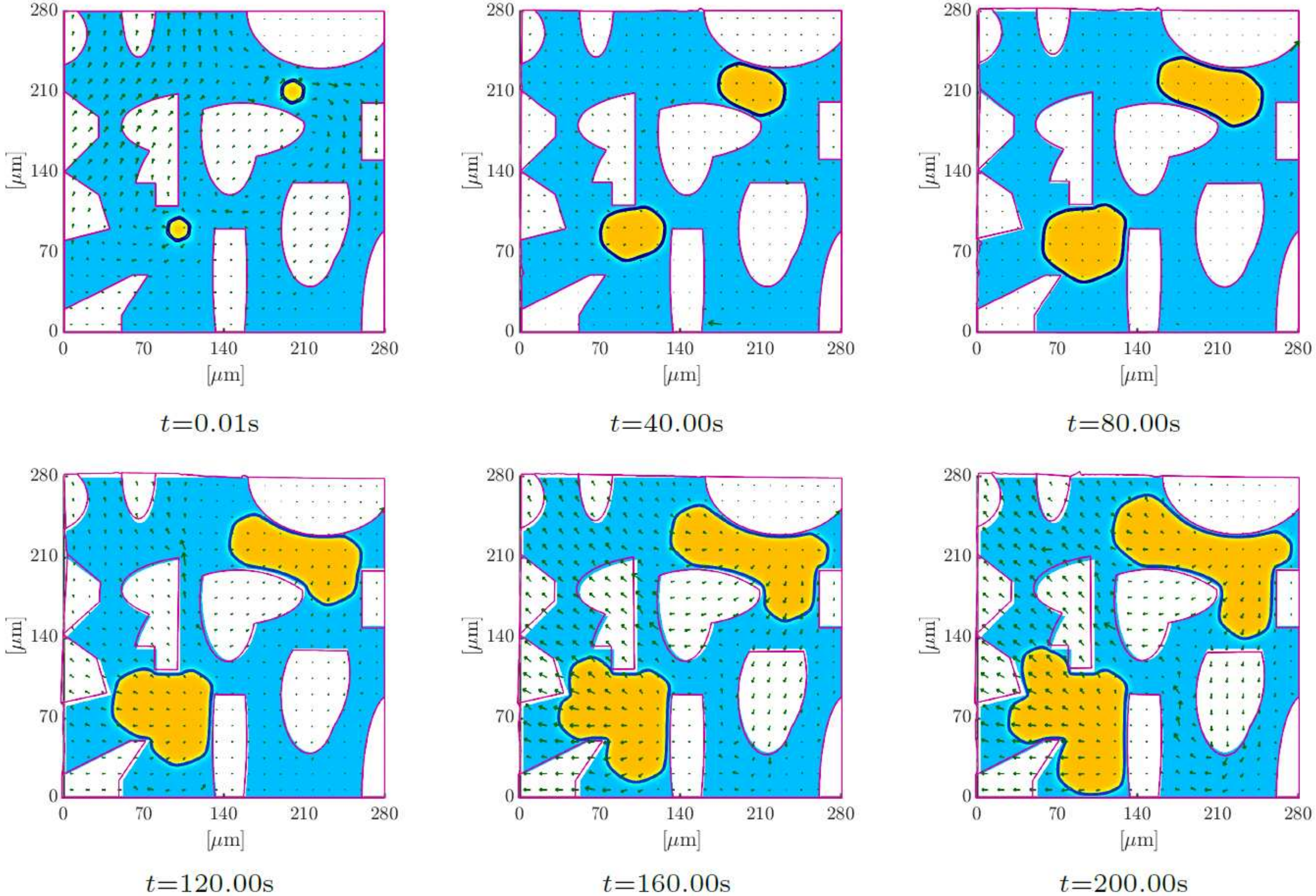



Temperature distribution

Formation of solid phase in complex pore geometry

Nucleation site defined by the initial condition, scale is in $\mu$m

# **Computational Studies** - growth in pores - phase position




Pore filled by liquid (in blue) and solid (in yellow), structural changes oversized and indicated in green

Formation of solid phase in complex pore geometry

Nucleation site defined by the initial condition, scale is in $\mu$m