Environmental Modeling

Mathematical Model of Freezing in a Porous Medium at Micro-Scale

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Outline of the talk

1. Motivation and examples
2. Phenomenology of phase transition in porous media
   - energy balance
   - mechanical balance
   - phase tracking
   - density difference and simplifications
   - thermodynamical description
   - modified Stefan problem
   - thin layers
3. Conservation laws
   - mass
   - energy
   - momentum
4. Computational studies
   - macrosscale
   - microscale
5. Undergrad challenges

Acknowledgement

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Joint work:

- Colorado School of Mines (T.H. Illangasekare, A.C. Trautz)
- Faculty of Civil Engineering, CTU Prague (A. Žák, M. Sobotková, M. Sněhota)

Motivation

- thaw - freeze cycles in nature
- release of methane from permafrost - climate changes in arctic regions and consequences
- seasonal structural changes in constructions
- fabrication of advanced materials
- phase change energy storage

Examples - part I

frost heave - patterning at soil surface in regions affected by cold winter

rails after cold season

road after cold season

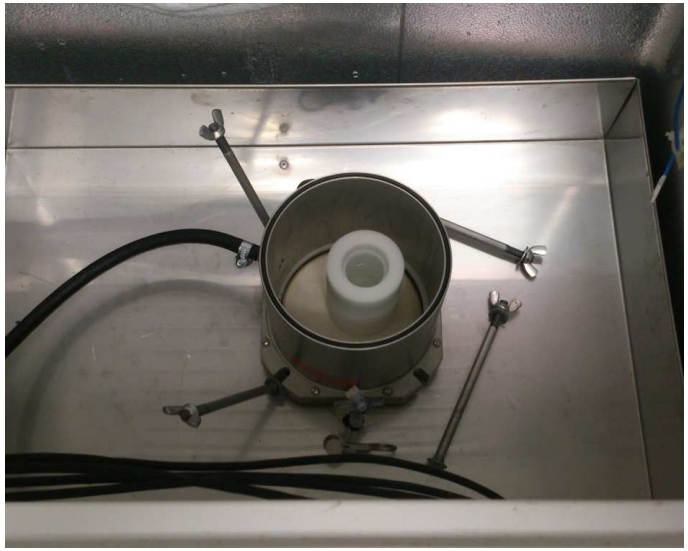
Examples - part II

methane gaps exploded after breaking the permafrost cap

broken permafrost layers

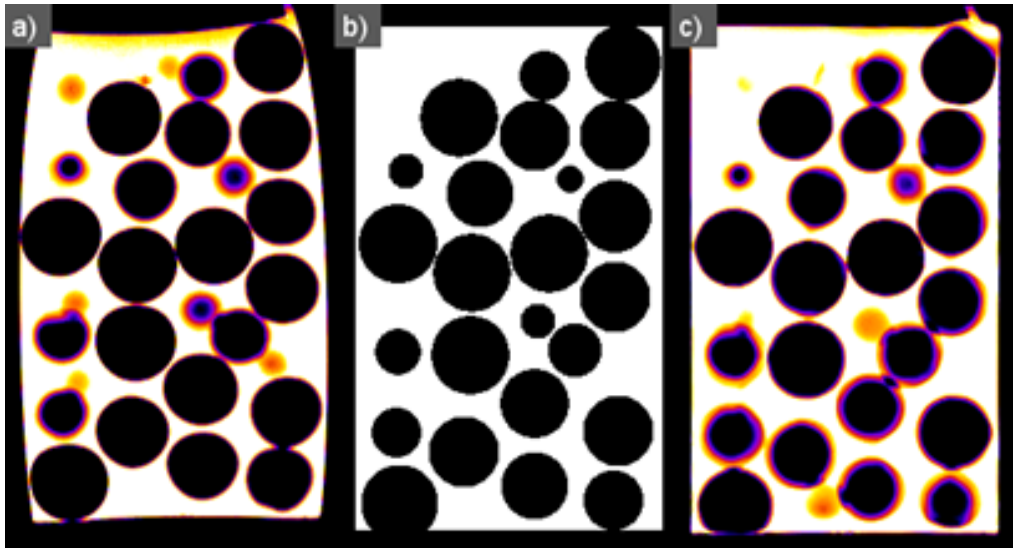
Experimental Evidence

coffe-cup experiment – measurements at CTU, Civil Engineering

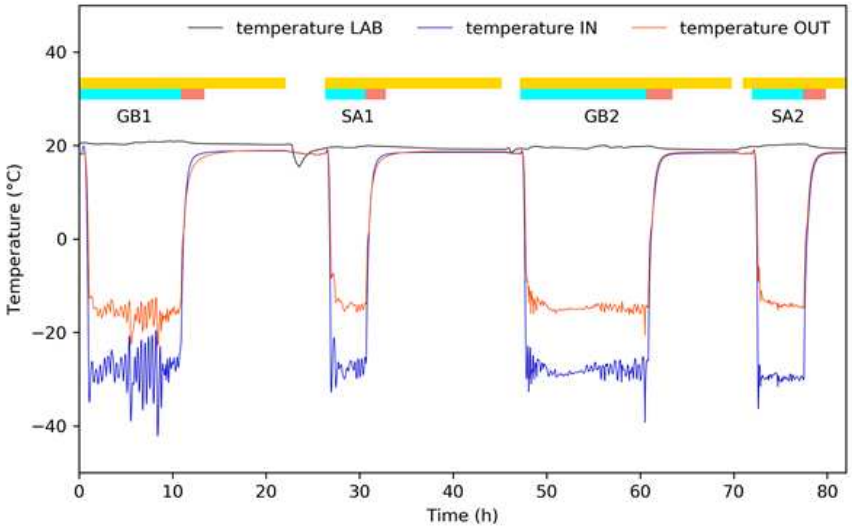


broken permafrost layers

Measurements



measurements at CTU, Civil Engineering



measurement of temperature

Phenomenology of Phase Transitions in Porous Media

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

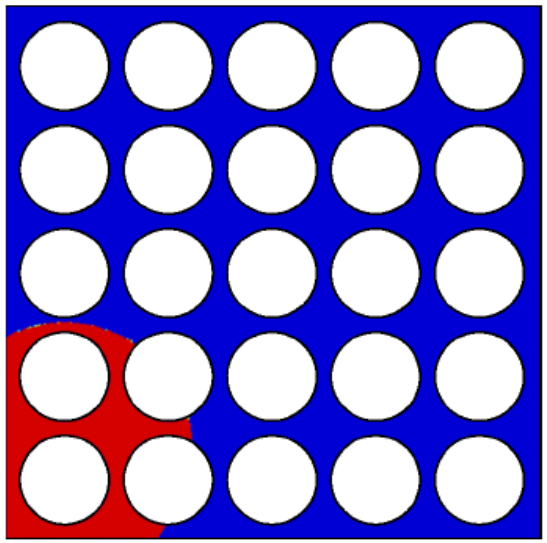
- Heat transfer - controlling mechanism
- Variations in specific volume in solid-liquid transition
- Induced forces causing deformation and motion
- Heterogeneous spatial structure
- High-curvature surface phenomena
- Gas dissolution in liquid and solid phases

Scales

$10^0 - 10^2$ m

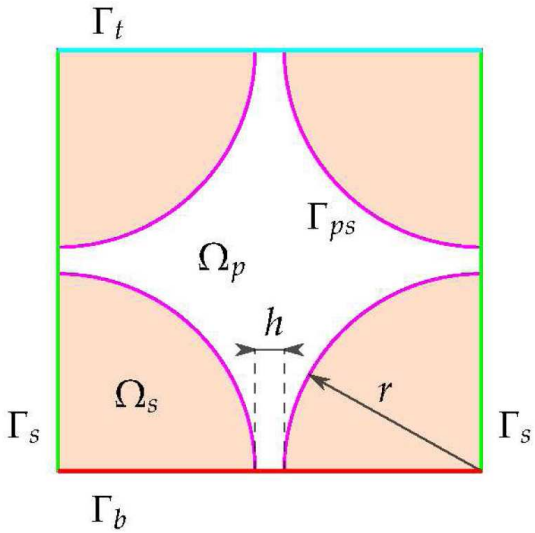
landscape

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



REV with many recognized pores

10^{-6} m



MED with a single pore

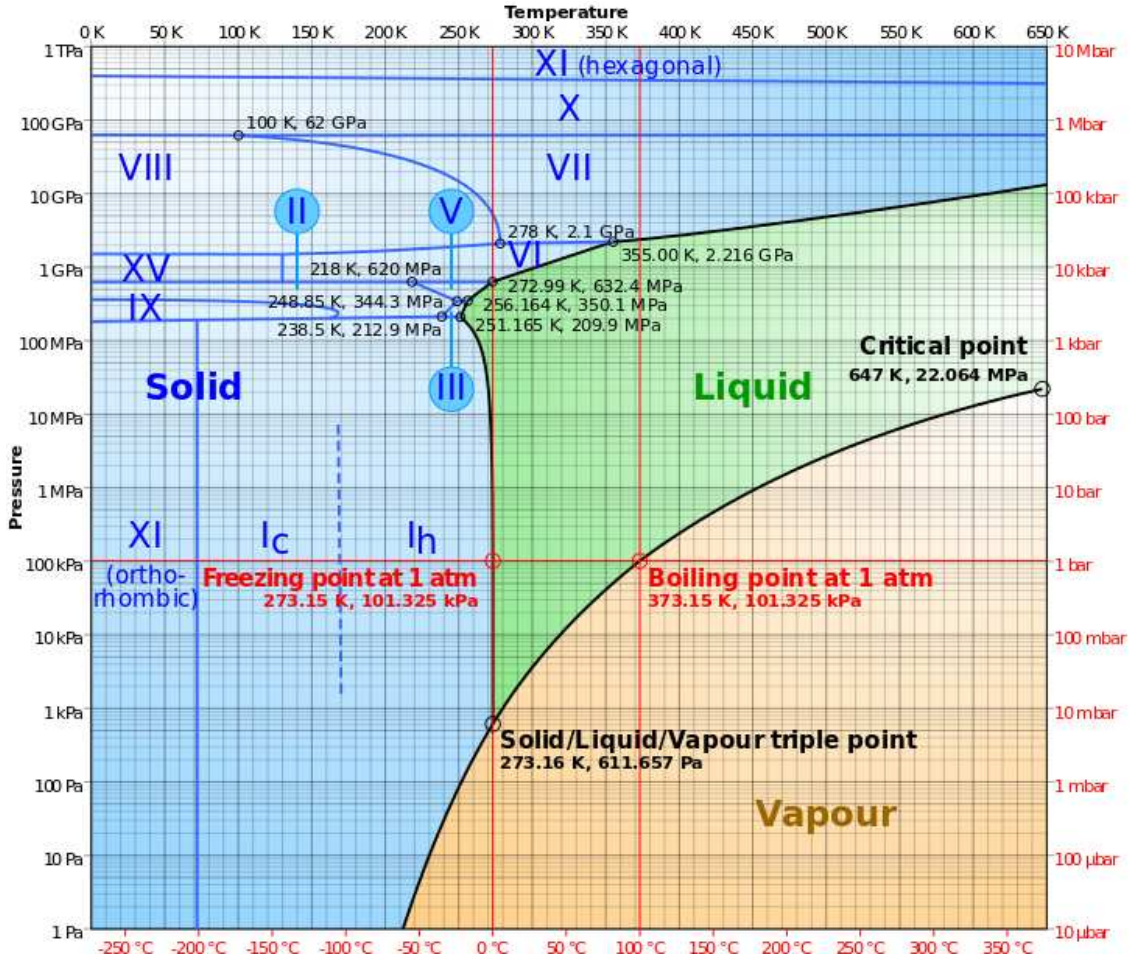
Phase Diagram

Clapeyron equation

$$\frac{dP}{dT} = \frac{L}{T\Delta v}$$

- P - thermodynamic pressure
- T - absolute pressure
- L - specific latent heat
- Δv - specific change in volume due to the phase change

Water Phase Diagram



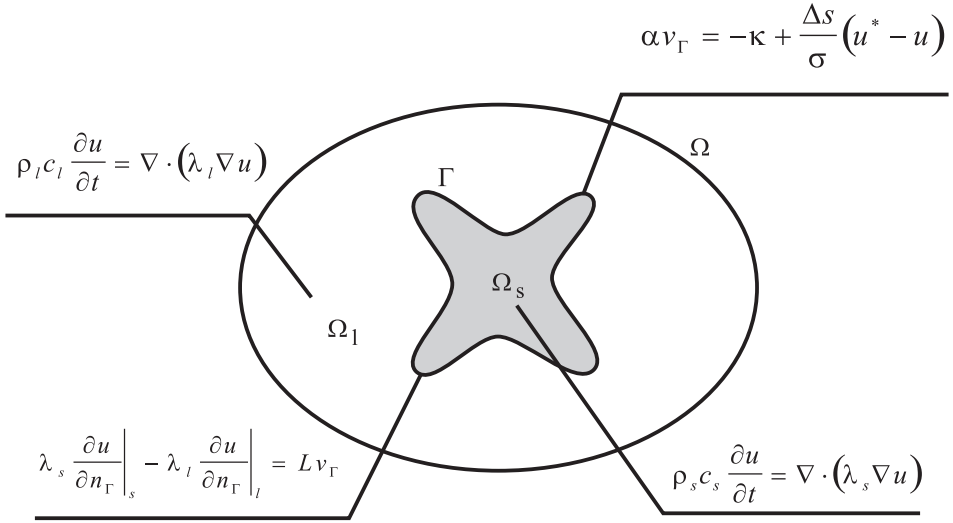
17 known ice phases

Stefan Problem with Surface Tension

Clapeyron equation incorporated into the energy balance at microscale

$$
\begin{aligned}
C\frac{\partial T}{\partial t} &= \nabla(k\nabla T) \text{ v } \Omega_s \text{ a } \Omega_l \\
b_c(T)\mid_{\partial\Omega} &= 0 \\
T\mid_{t=0} &= T_0 \\
k\frac{\partial T}{\partial n}\mid_s - k\frac{\partial T}{\partial n}\mid_l &= Lv_\Gamma \\
T - T^* &= -\frac{\sigma}{\Delta s}\kappa_\Gamma - \alpha\frac{\sigma}{\Delta s}v_\Gamma \\
\Omega_s(t)\mid_{t=0} &= \Omega_{so}
\end{aligned}
$$

$\lambda_s,\ \lambda_l$	heat conductivity
$\sigma = f(T^*)$	surface tension
κ_Γ	mean curvature of the hypersurface $\Gamma(t)$
$\mathbf{n}_\Gamma$	normal unit vector to $\Gamma(t)$ pointing out of Ω_s
v_Γ	normal velocity of $\Gamma(t)$
$\mathbf{n}_{\partial\Omega}$	normal unit vector to $\partial\Omega$ pointing out of Ω
$\Omega_L(t),\ \Omega_S(t)$	liquid/solid subdomain
$T = T(t,x)$	temperature
L	latent heat



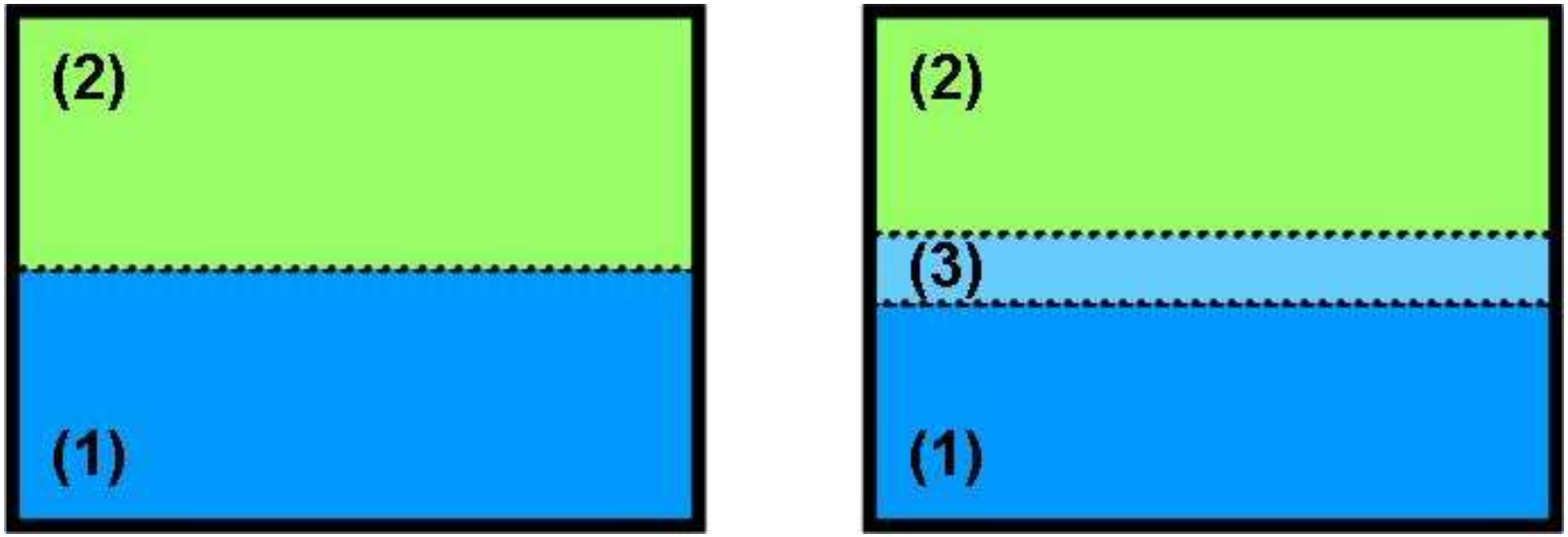
Dirichlet boundary condition :

$$b_c(T)\mid_{\partial\Omega} = u\mid_{\partial\Omega} - g_0$$

or Neumann boundary condition:

$$b_c(T)\mid_{\partial\Omega} = \frac{\partial u}{\partial n}\mid_{\partial\Omega} - g_1$$

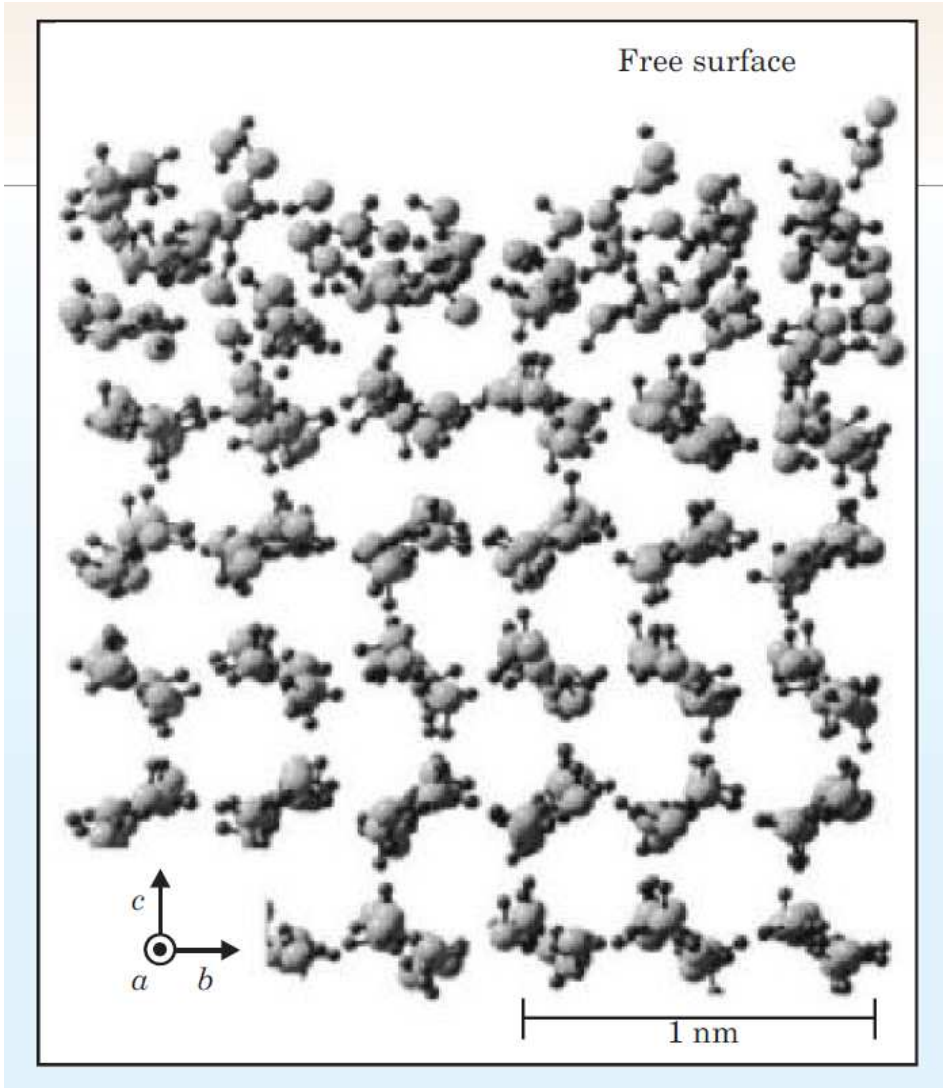
Thin Liquid Layers



Layered structures of phase interface (1) = ice, (2) = grain, (3) = liquid

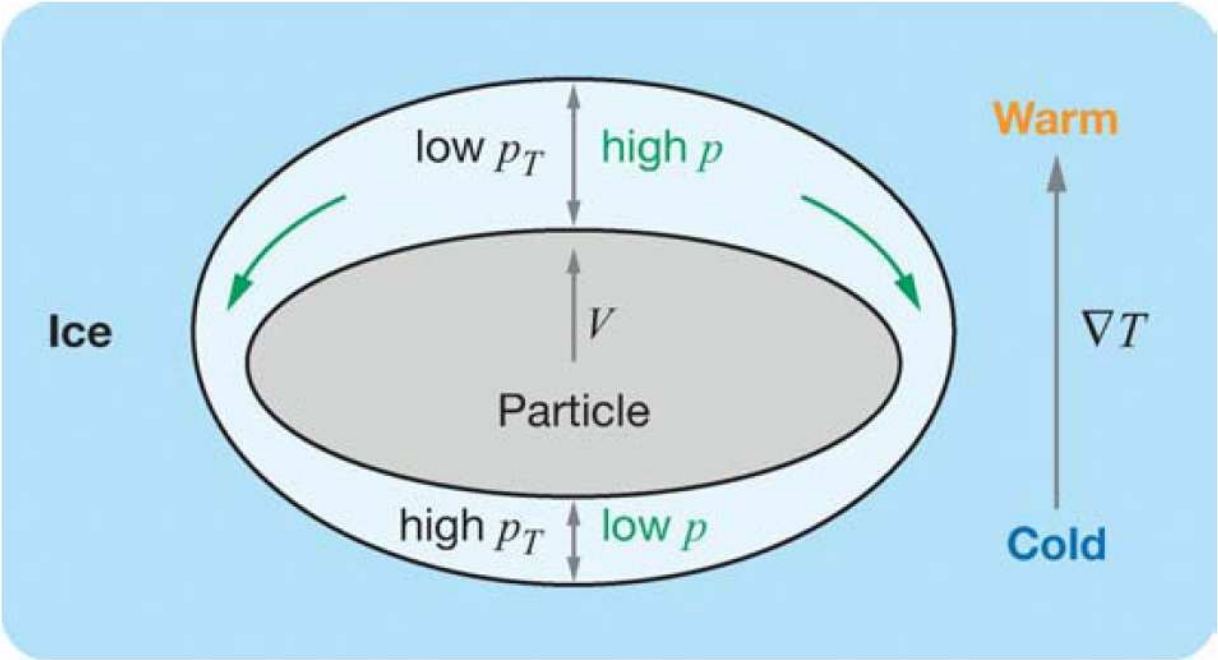
Liquid layer occurs when **surface tensions** of solid/liquid + liquid/grain < solid/grain

Thin Layer Understanding



Disordered upper layer of water molecules

Premelting 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.

Poromechanics

Assuming linear elasticity and very small displacements

Strain in Ω_G and Ω_P

$$\epsilon_{ij}^{el} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

Stress by Hook's law in Ω_G

$$\sigma_{ij} = \frac{E_G}{1+\nu}\left(\epsilon_{ij}^{el} + \frac{\nu}{1-2\nu}\epsilon_{kk}^{el}\delta_{ij}\right)$$

Stress expression with expansivity in Ω_P

$$\sigma_{ij} = \frac{E_P(p)}{1+\nu}\left(\epsilon_{ij}^{el} + \frac{\nu}{1-2\nu}\epsilon_{kk}^{el}\delta_{ij}\right) + F_{exp}(p)\mathbb{I}$$

where

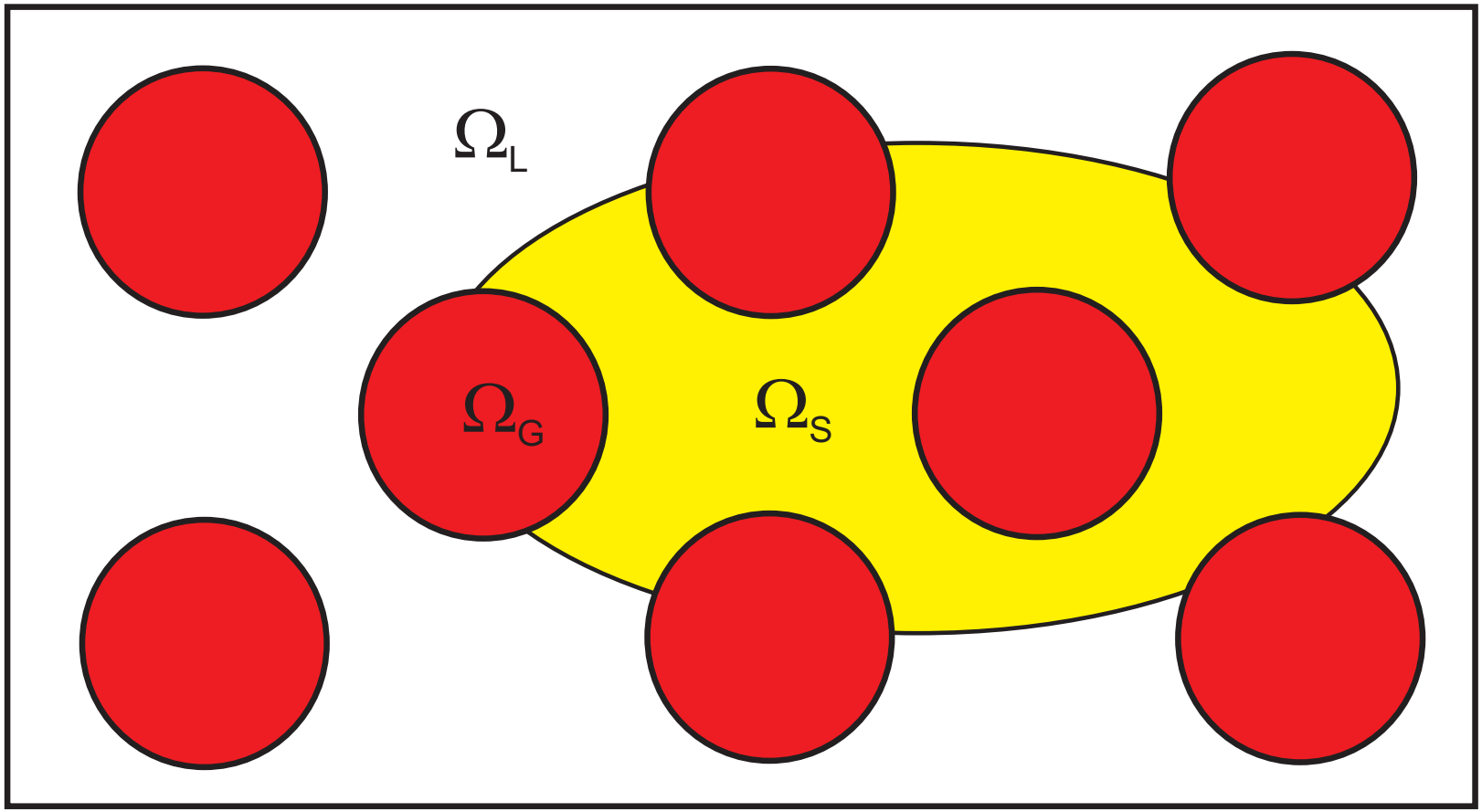
$$E_G = const., \qquad E_P(p) = pE_{melt} + (1-p)E_{solid}, \qquad F_{exp}(p) = c_{exp}p$$

Newton's force balance law

$$\varrho\frac{\partial^2 u_i}{\partial t^2} - \frac{\partial \sigma_{ij}}{\partial x_j} = 0$$

with natural boundary conditions and with continuity of displacement and derivatives across $\Omega_G \cap \Omega_P$

Conservation Laws - geometry



Space domain consists of grains Ω_G and pores filed by liquid Ω_L and solidified phase Ω_S

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

Conservation Laws - general

Volume balance

$$\dot{\bar{\phi}}(t,x) + \phi(t,x)\nabla\cdot\mathbf{v}(t,x) + \nabla\cdot\xi(t,x) - \Sigma(t,x) = 0 \quad \text{in } \mathcal{V} - \mathcal{S}(t)$$

Interface balance

$$[\![\phi(t,x)(\mathbf{v}(t,x) - \mathbf{u}(t,x)) - \xi(t,x)]\!]\cdot\mathbf{n} = 0 \quad \text{on } \mathcal{S}(t)$$

- $\dot{\bar{\phi}}$ - material derivative of quantity ϕ
- $\mathbf{v}(t,x)$ - velocity of material point
- $\xi(t,x)$ - surfacial flux of quantity ϕ
- $\Sigma(t,x)$ - volumic source density of quantity ϕ
- $\mathcal{V}$ - investigated volume
- $\mathcal{S}(t)$ - boundary moving with velocity $\mathbf{u}(t,x)$
- $\mathbf{n}$ normal vector to $\mathcal{S}(t)$

Applied to:

- mass described by mass density ϱ
- momentum described by momentum density $\varrho\mathbf{v}$
- energy described by internal energy density and characterized by absolute temperature T

Conservation Laws - constitutive relations

Stress in grain matrix

$$\sigma_{ij} = \frac{E_G}{1+\nu}\left(\epsilon_{ij}^{el} + \frac{\nu}{1-2\nu}\epsilon_{kk}^{el}\delta_{ij}\right), \quad \epsilon_{ij}^{el}(t,x) = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

Stress in solid phase

$$\sigma_{ij} = \frac{E_S}{1+\nu}\left(\epsilon_{ij}^{el} + \frac{\nu}{1-2\nu}\epsilon_{kk}^{el}\delta_{ij}\right) + \beta\delta_{ij}$$

where β is the volume expansion factor

Stress in Newtonian incompressible liquid phase

$$\sigma_{ij} = -p(t,x)\delta_{ij} + 2\mu\mathbf{d}_{ij}(t,x), \quad \mathbf{d}_{ij}(t,x) = \frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)$$

Fourier law for heat flux and expression for internal energy of solid

$$\xi_{heat} = -k\nabla T, \qquad u(t,x) = \int_{T_0}^{T} C(T)\mathrm{d}T$$

where k is heat conduction coefficient, c is specific heat capacity

Enthalpy of liquid including latent heat L

$$h(t,x) = u(t,x) + L$$

Macro-Scale Model

Designed for large macroscale, based on empirical melting point depression by pores with high-curvature boundaries

Heat conduction with empirical latent heat source term

$$C\frac{\partial T}{\partial t} + L\frac{\partial \theta(T)}{\partial t} = \nabla \cdot (k\nabla T), \quad \theta(T) = \begin{cases} \eta & \text{for } T \geq T^D \\ \eta \left| \dfrac{T^D - 273.15}{T - 273.15} \right|^b & \text{for } T < T^D \end{cases}$$

where - η is porosity, $T^D < 273.15$ melting point depression, $b > 0$ empirical constant

Momentum balance at large scale (homogenized)

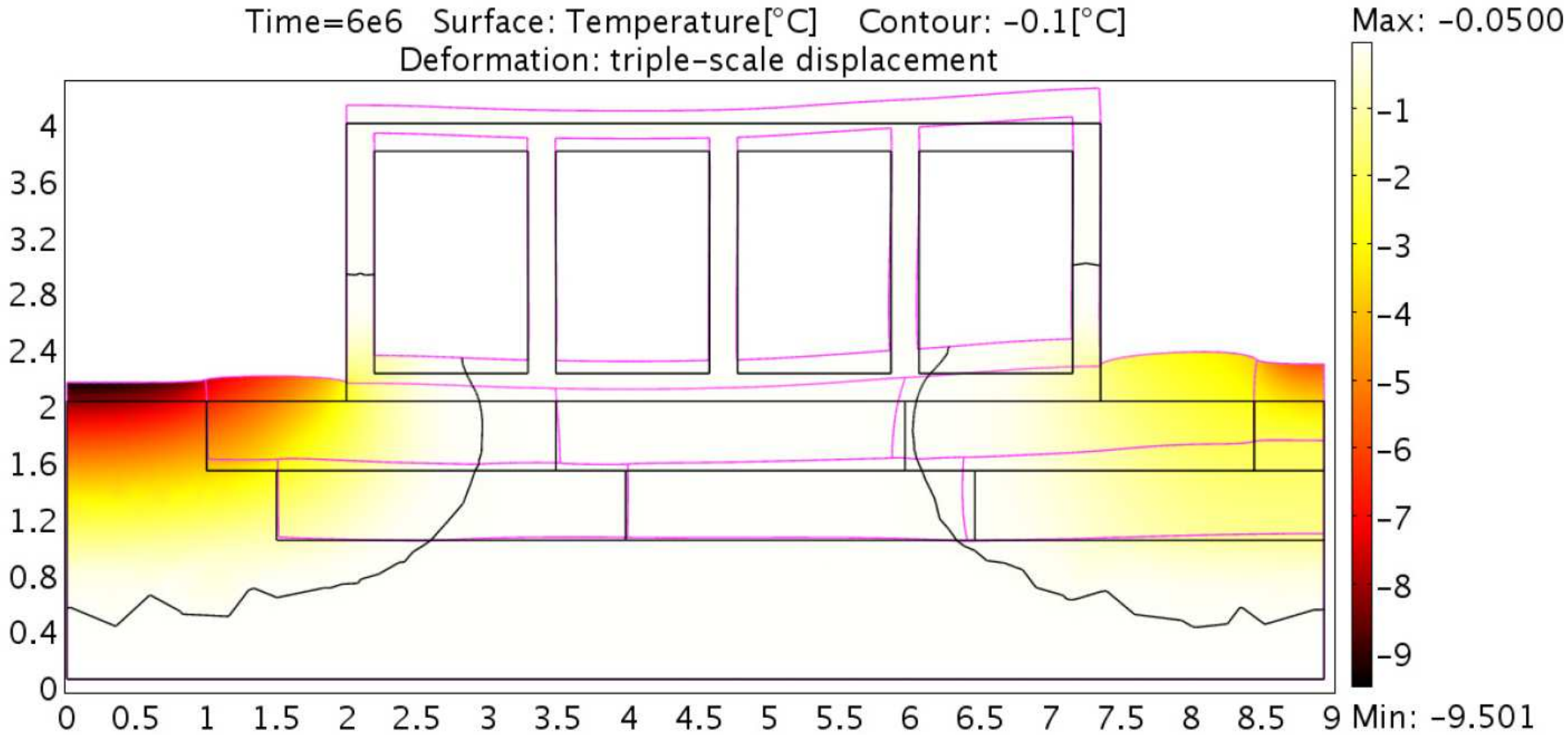
$$\varrho \frac{\partial^2 u_i}{\partial t^2} - \frac{\partial \sigma_{ij}}{\partial x_j} = 0$$

$$\sigma_{ij} = \frac{E}{1+\nu}\left(\epsilon_{ij}^{el} + \frac{\nu}{1-2\nu}\epsilon_{kk}^{el}\delta_{ij}\right) + \beta(T)\delta_{ij}, \quad \beta = \begin{cases} \bar{\beta} & \text{for } T \leq T^D \\ 0 & \text{for } T > T^D \end{cases}$$

Reference and with references therein:

Žák A., Beneš M. and Illangasekare T. H. Analysis of Model of Soil Freezing and Thawing. *IAENG International Journal of Applied Mathematics*, Volume 43, Issue 3, pp. 127–134, September 2013

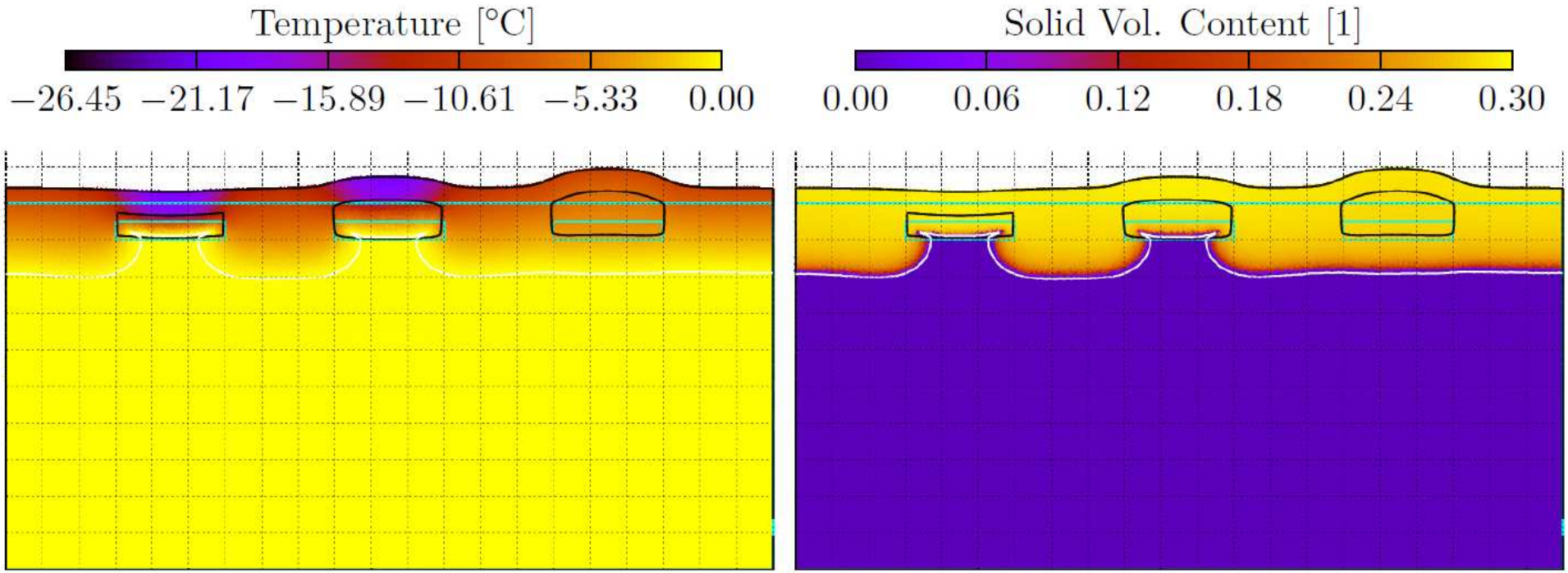
Macro-Scale Computational Studies - building heave



Strain evolution of the concrete construction during ground soil freezing

An illustrative example explaining purpose of modeling

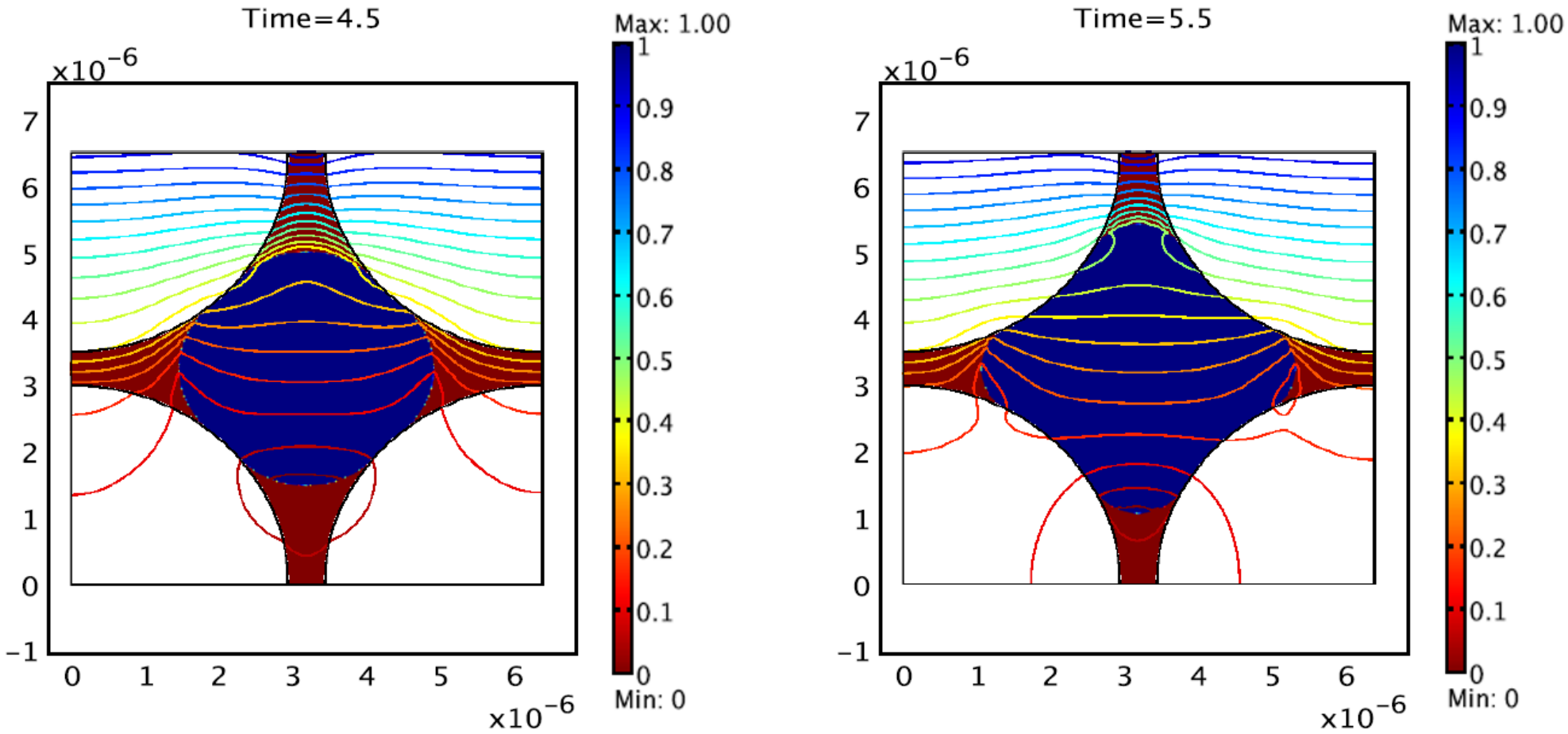
Macro-Scale Computational Studies - vertical soil behavior



(a) $t = 40$[h]

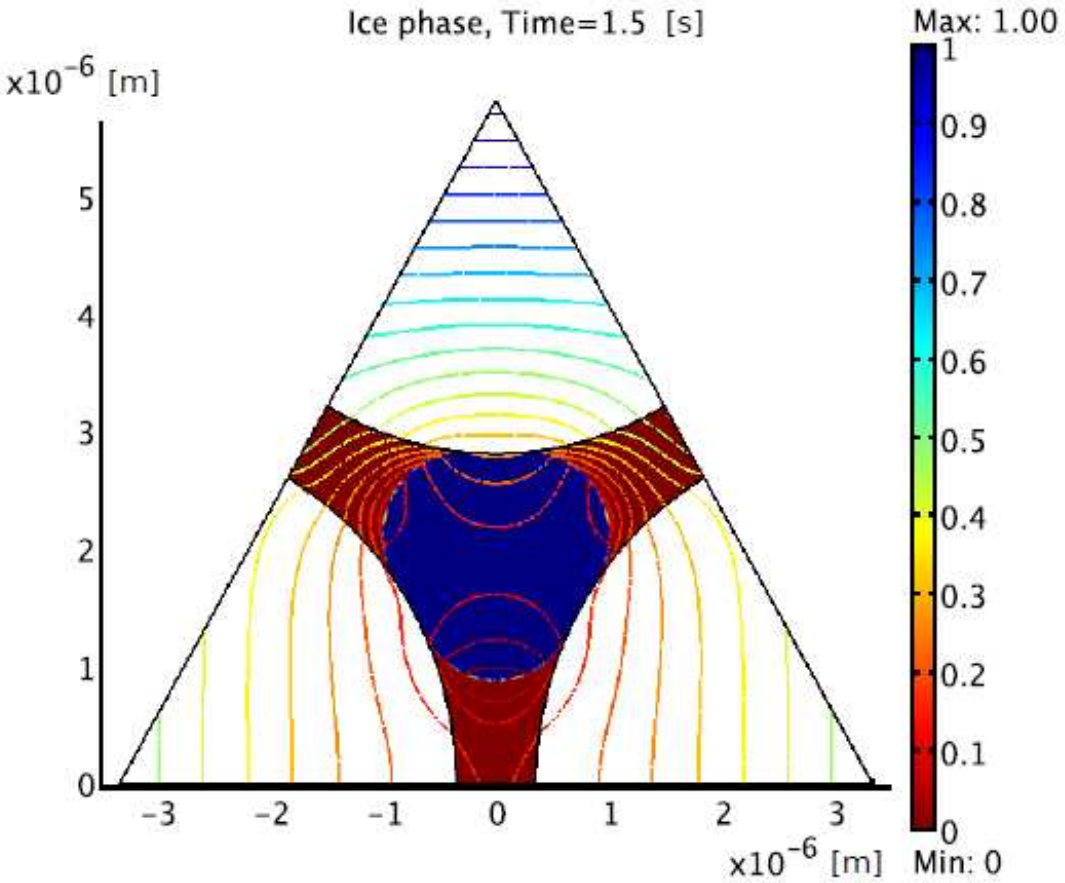
Vertical heterogeneous soil structure filled by liquid and solid phase with indication of temperature at a particular time moment. Cooling set from above. Domain deformation visually magnified.

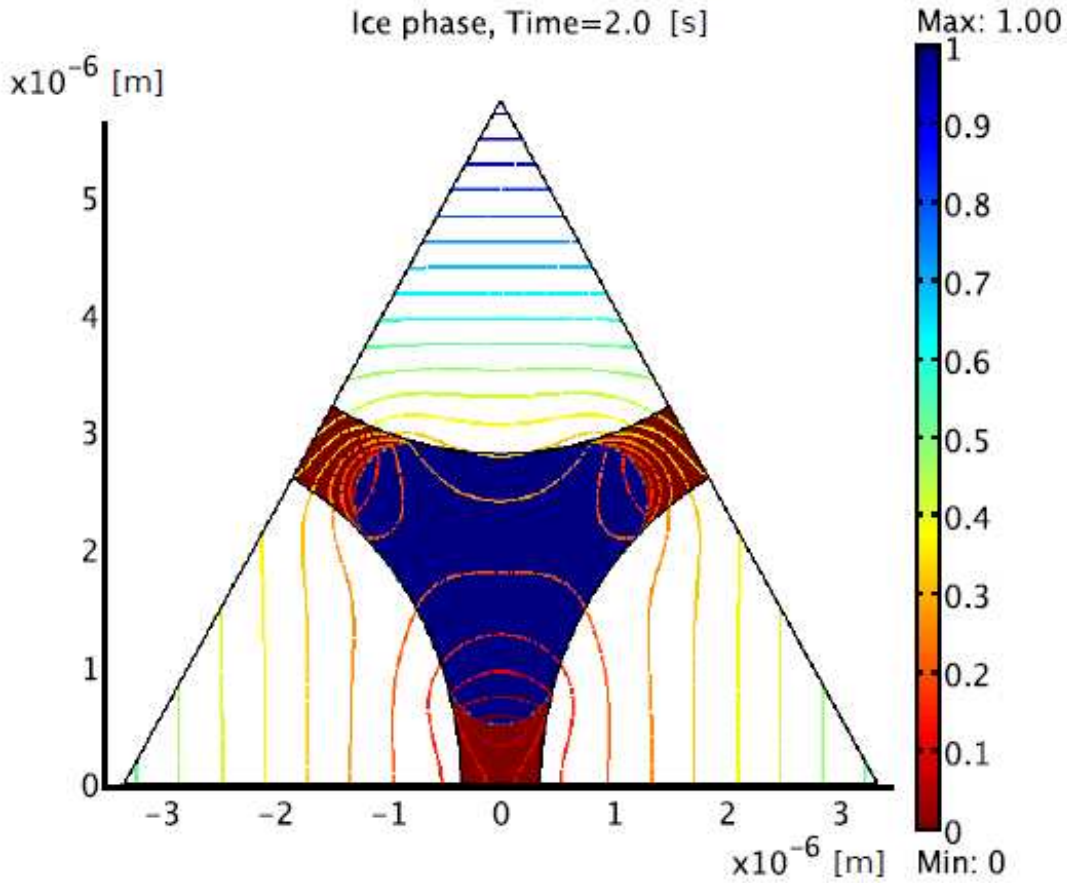
Symmetric Micro-Scale Model - results 1



Temperature distribution in a symmetric pore domain under vertical external temperature gradient

Symmetric Micro-Scale Model - results 2





Solidification in a triangular symmetric pore domain under vertical external temperature gradient

Phase-Field Micro-Scale Model

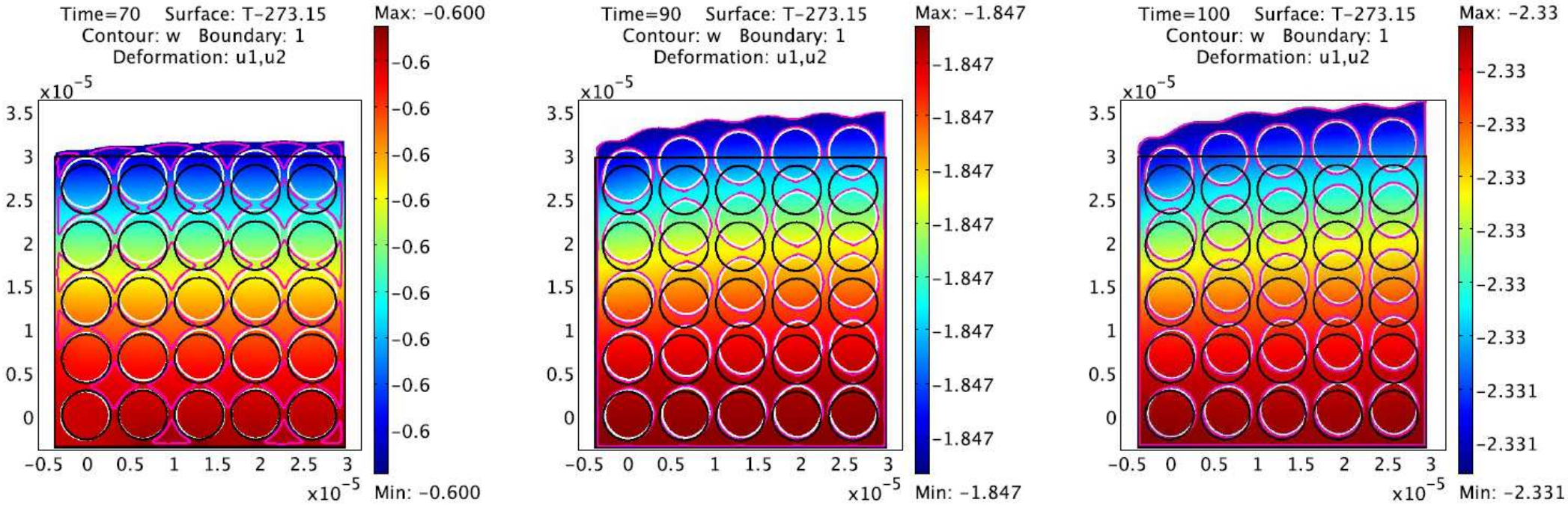
Derived for representative microscale on a general pore domain.

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

Reference:

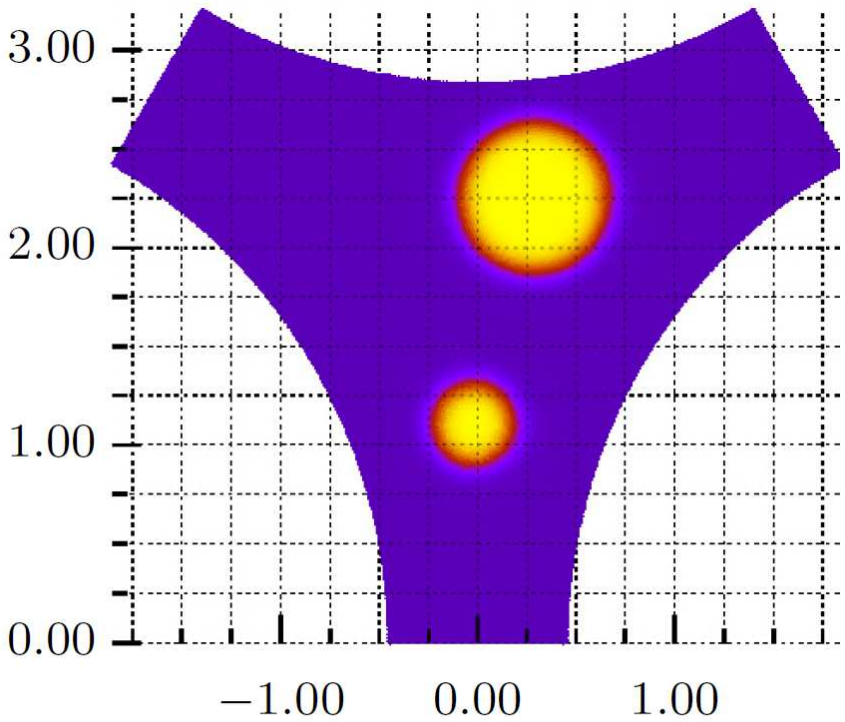
Žák A. and Beneš M. Micro-Scale Model of Thermomechanics in Solidifying Saturated Porous Media, *Acta Physica Polonica* 134 (3), 2018, pp. 678–682.

Computational studies - small pack

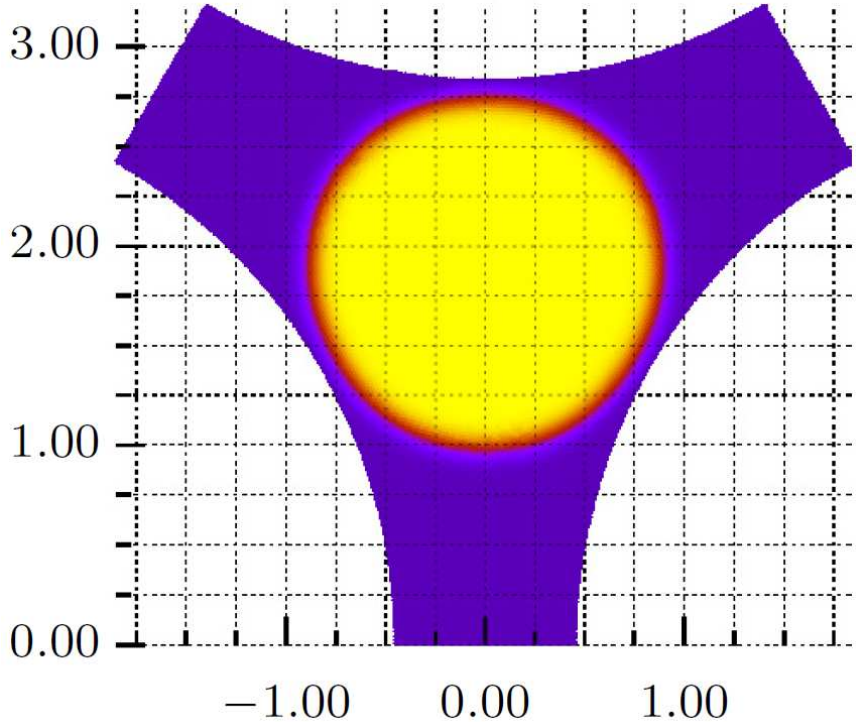


Color scale indicates distribution of temperature at selected time moments $t = 70$, $t = 90$ and $t = 100$

Computational Studies - part 1



(d) $w_{\text{ini}} = w_9$, $t = 7.5\times10^{-3}$[s]



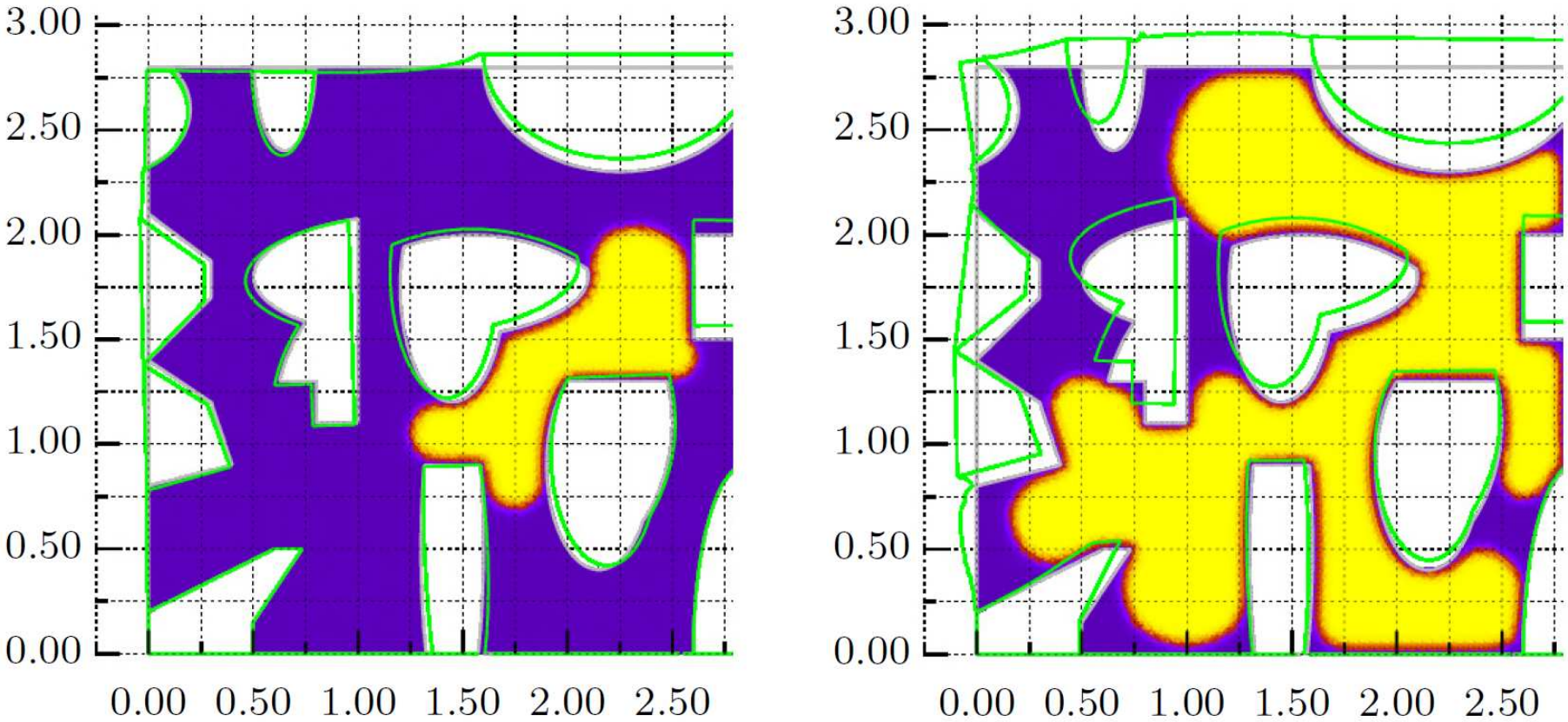
(f) $w_{\text{ini}} = w_9$, $t = 0.95$[s]

Pore filled by liquid (in blue) and solid (in yellow)

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

Computational Studies - part 2



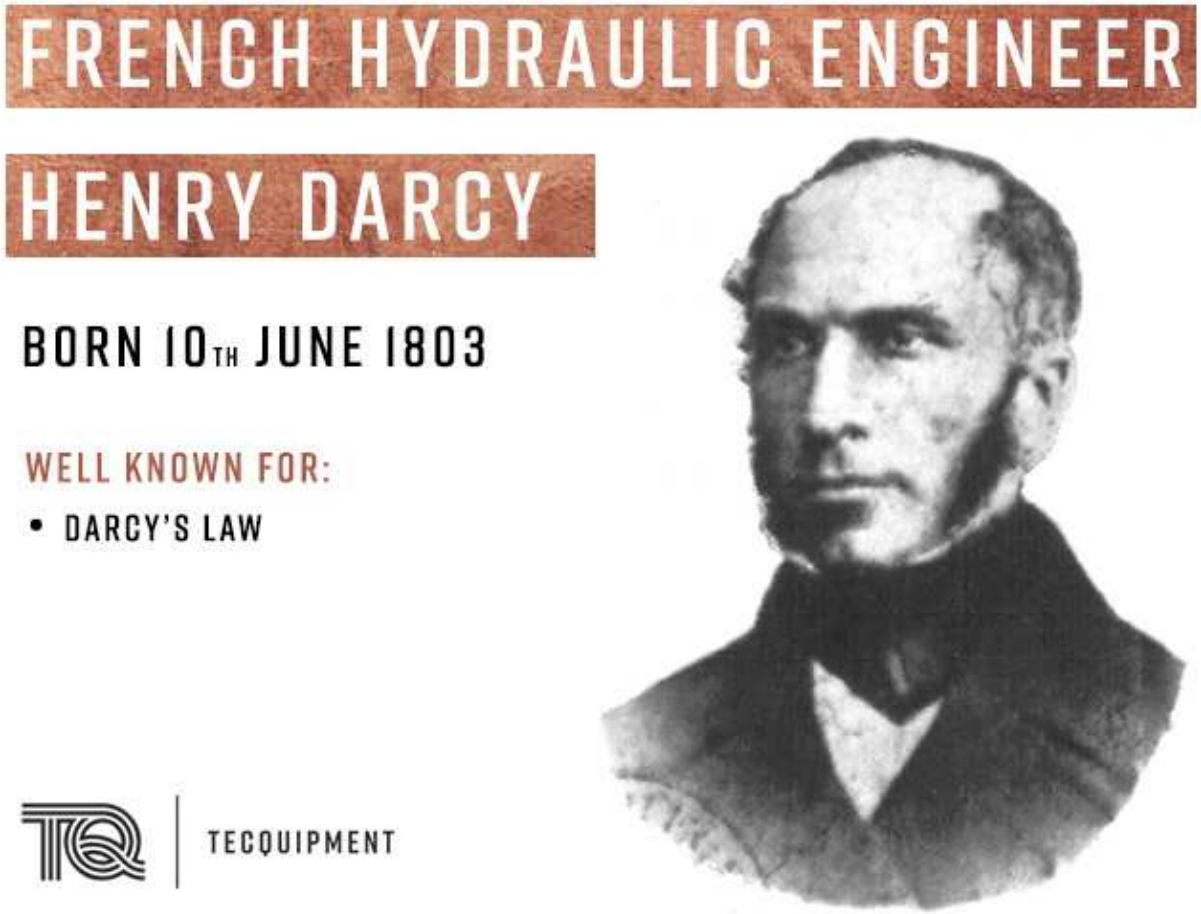
(a) $t = 80[\mathrm{s}]$ (f) $t = 380[\mathrm{s}]$

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

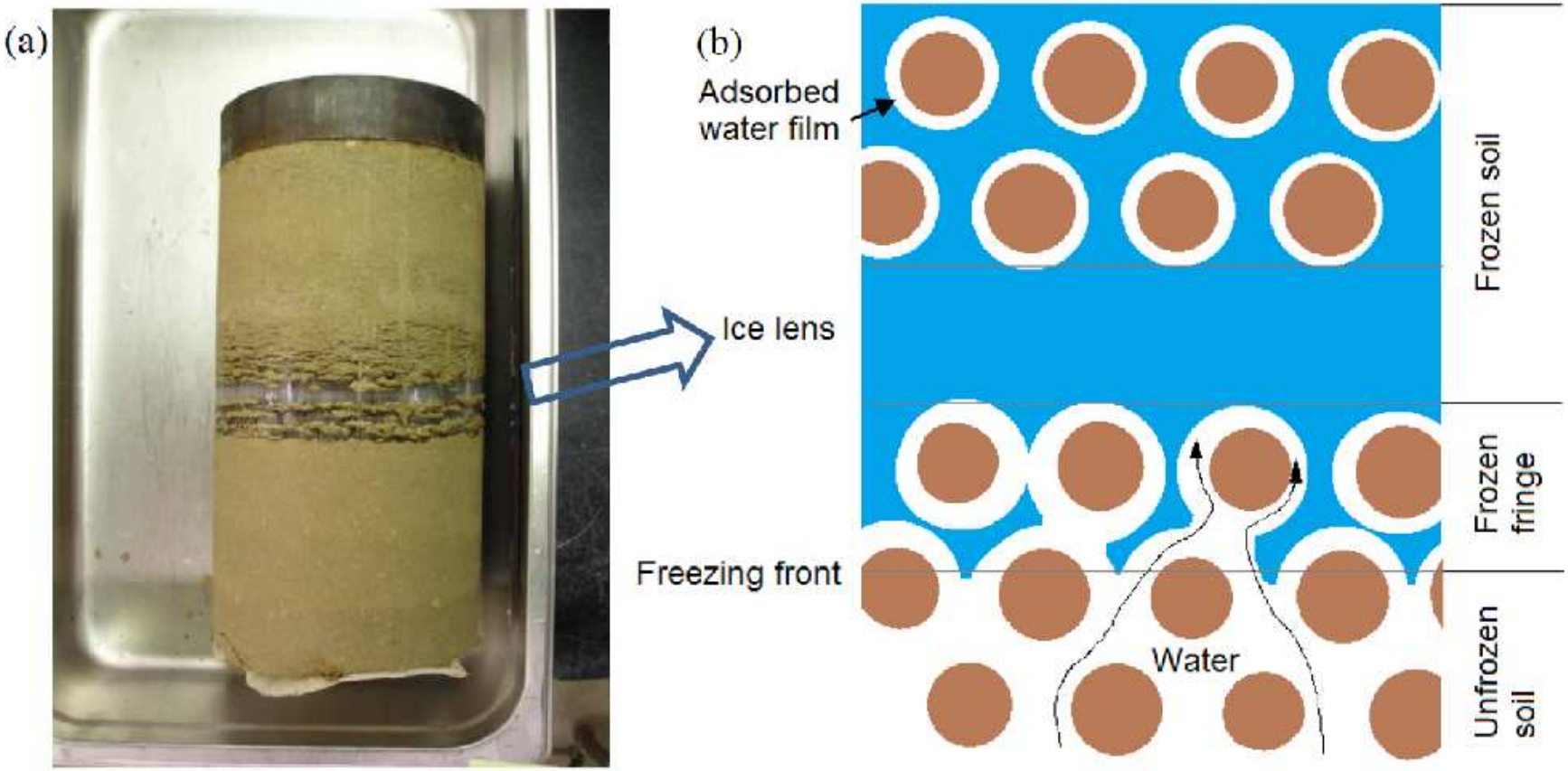
Challenges - for undergrads I



Gas release from porous media - multiphase flow described by the Darcy law.

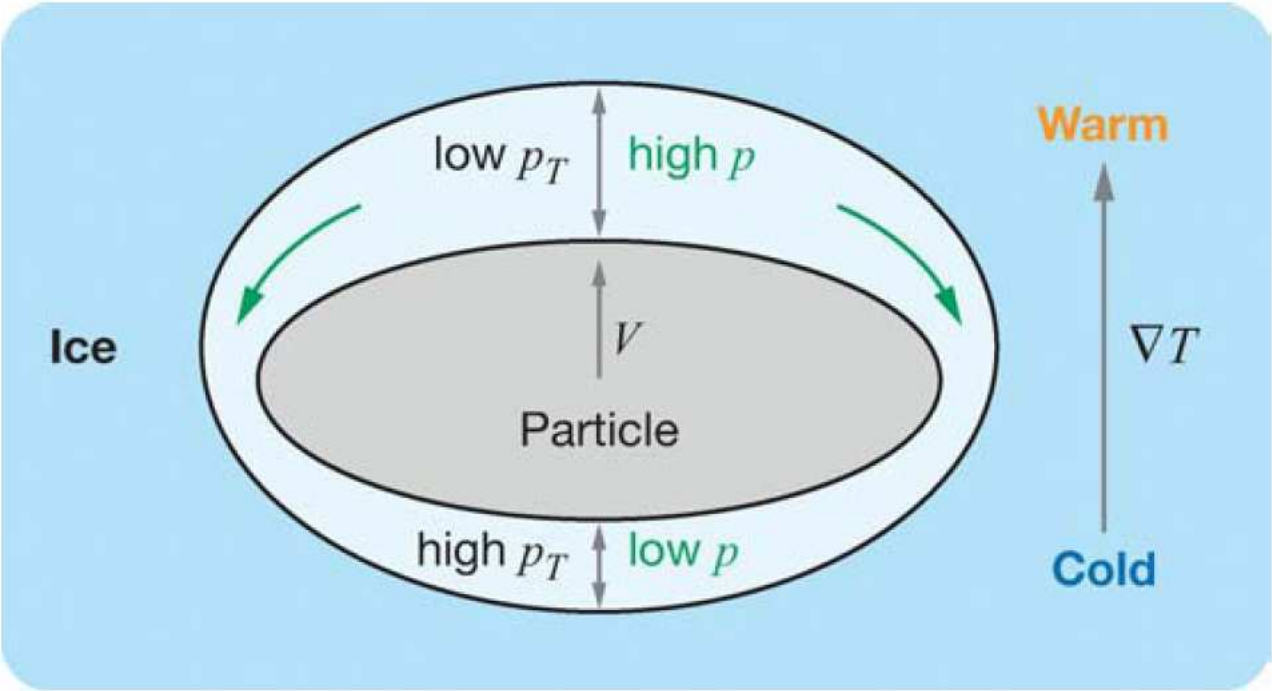
$$\mathbf{j}_\alpha = -\mathbb{K}_\alpha \nabla p_\alpha, \quad \text{for the phase } \alpha$$

Challenges - for undergrads II



Modeling the frost heave during soil freezing.

Challenges - for undergrads III



Transport along surfaces during soil freezing.

Question

Henry's law for maximum gas concentration solvable in a liquid

$$C = H \ \exp(Q(\frac{1}{T} - \frac{1}{T_{ref}}))Mp$$

- $C \ kg/m^3$ - gas concentration
- $p \ Pa$ - gas pressure
- $T \ K$ - system temperature
- $H \ mol/m^3/Pa$ - Henry's constant
- $M \ kg/mol$ - molar gas mass
- $Q \ K$ - constant

For argon at $p = 3atm = 300kPa$ is maximum concentration $0.147kg/m^3$, i.e. the experimental container of $28ml$ has maximum of $4.129mg$ of argon.