Department MATHEMATIK

FAU FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG

NATURWISSENSCHAFTLICHE FAKULTÄT

Micro-macro models for reactive two-mineral systems

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Motivation

Evolving structures

- at the pore scale by means of **heterogeneous precipitation/dissolution reactions**
  $\Rightarrow$ Change of flow path and macroscopic hydrodynamic properties
- Three-phase system with two solid phases instead of three-phase system with two liquid phases
- **Level-set approach** instead of phase-field approach

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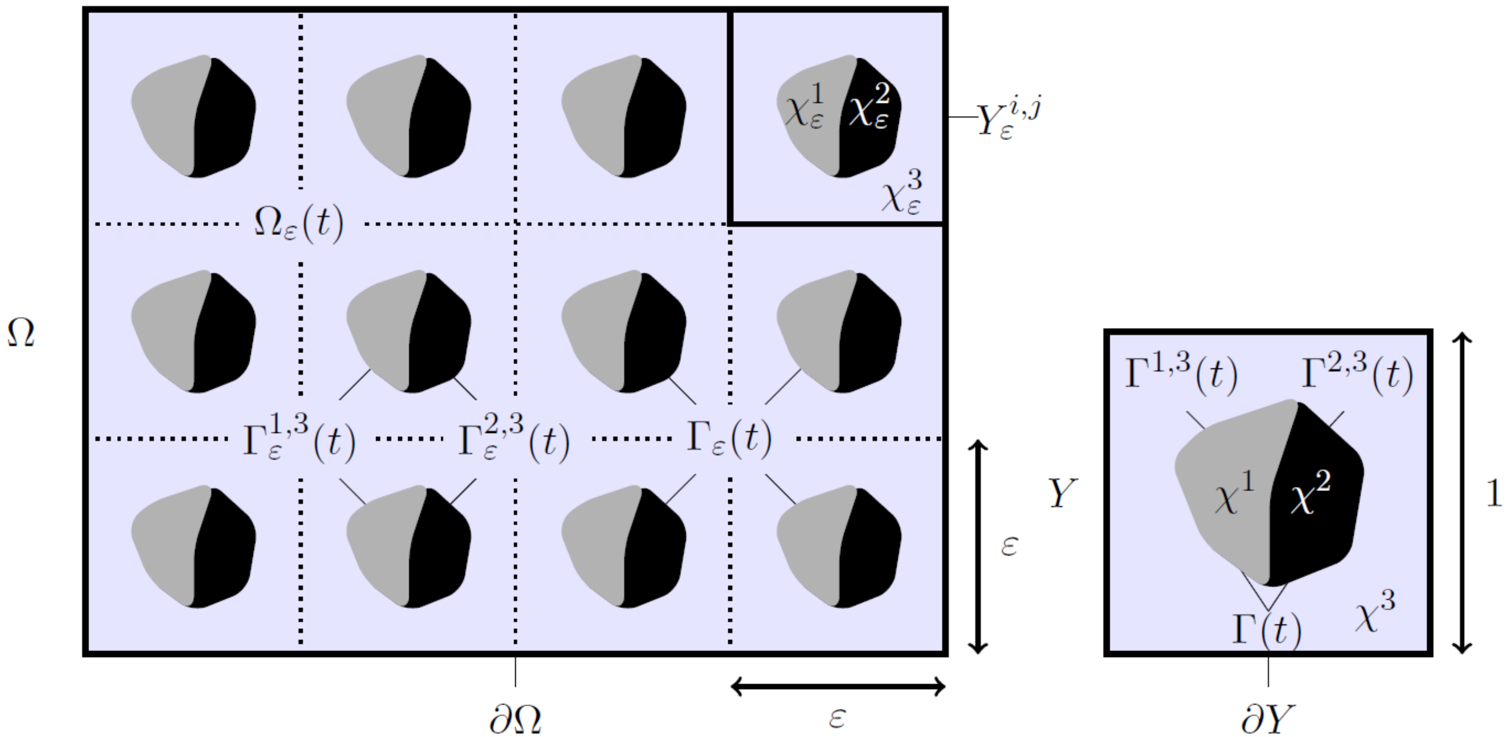
- **Level-set approach** instead of phase-field approach

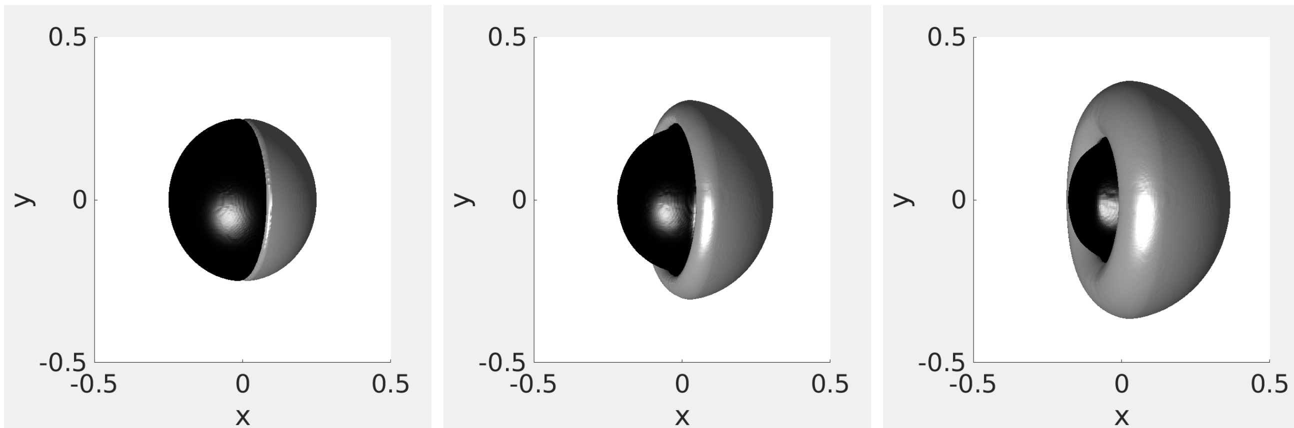
Reactive flow and transport modeling on different scales

- **Multiscale models (obtained by averaging)**

Pore-scale model in evolving domain – geometrical setting



Pore-scale model in evolving domain – level set approach



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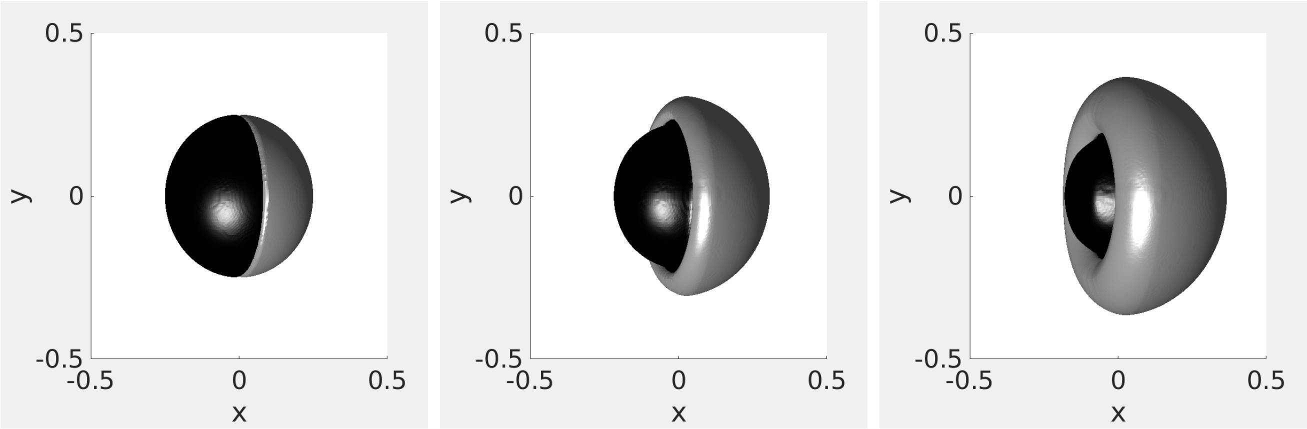

Level set is capable characterizing fluid–solid interface

$L_\varepsilon(t,x) < 0$ in fluid phase/pore space,
$L_\varepsilon(t,x) = 0$ on solid–fluid interface,
$L_\varepsilon(t,x) > 0$ in solid phase.

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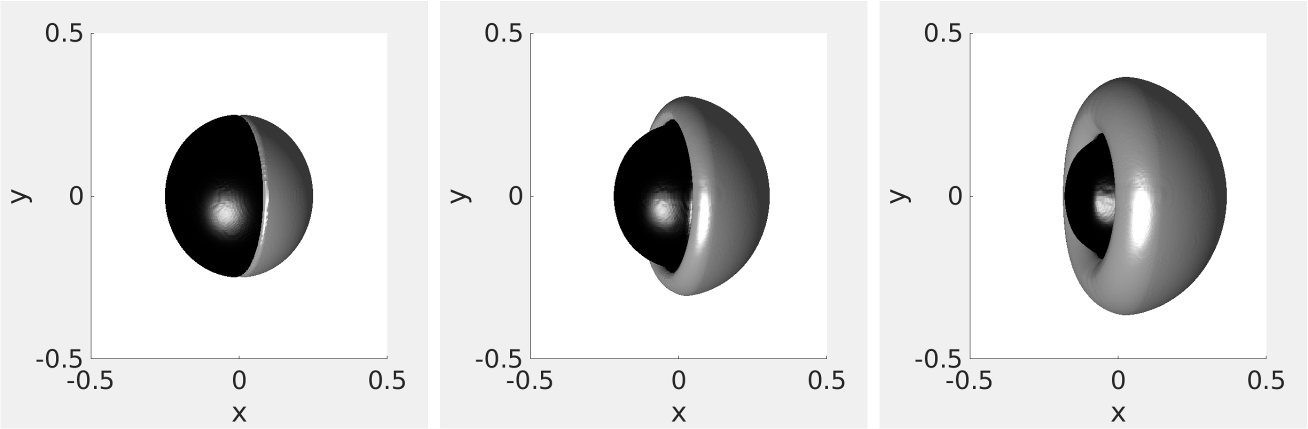

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Level set equation for level set L

$$\partial_t L_\varepsilon + v_{n,\varepsilon}|\nabla L_\varepsilon| = 0 \qquad x \in \Omega$$

with normal velocity of the interface $v_{n,\varepsilon}$ related to distinct reaction kinetics.

Pore-scale model in evolving domain – reactive flow and transport

Transport equation for concentration c_ε

$$
\begin{aligned}
\partial_t c_\varepsilon - \nabla \cdot (-v_\varepsilon c_\varepsilon + D_m \nabla c_\varepsilon) &= 0, && x \in \Omega_\varepsilon(t), t \in (0,T), \\
(-v_\varepsilon c_\varepsilon + D_m \nabla c_\varepsilon) \cdot \nu_\varepsilon - \varepsilon \alpha_1 f_1(c_\varepsilon, \rho_1)(c_\varepsilon - \rho_1) &= 0, && x \in \Gamma_\varepsilon^{1,3}(t),\ t \in (0,T), \\
(-v_\varepsilon c_\varepsilon + D_m \nabla c_\varepsilon) \cdot \nu_\varepsilon - \varepsilon \alpha_2 f_2(c_\varepsilon, \rho_2)(c_\varepsilon - \rho_2) &= 0, && x \in \Gamma_\varepsilon^{2,3}(t),\ t \in (0,T),
\end{aligned}
$$

with molecular diffusion D_m, interface normal ν_ε, reaction $f_i(c_\varepsilon, \rho)$, mineral densities ρ_i, and $\alpha_i = 1/\rho_i$, $i = 1, 2$.

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Stokes equation for advective velocity v_ε and pressure p_ε

$$\begin{aligned}
\varepsilon^2 \mu \Delta v_\varepsilon - \nabla p_\varepsilon &= 0, && x \in \Omega_\varepsilon(t), && t \in (0,T),\\
\nabla \cdot v_\varepsilon &= 0, && x \in \Omega_\varepsilon(t), && t \in (0,T),\\
v_\varepsilon &= \varepsilon \alpha_1 f_1(c_\varepsilon, \rho_1)\nu_\varepsilon, && x \in \Gamma_\varepsilon^{1,3}(t), && t \in (0,T),\\
v_\varepsilon &= \varepsilon \alpha_2 f_2(c_\varepsilon, \rho_2)\nu_\varepsilon, && x \in \Gamma_\varepsilon^{2,3}(t), && t \in (0,T).
\end{aligned}$$

with dynamic viscosity μ.

Porescale model in evolving domain – regularization

Interpolation of discontinuous reaction kinetics $\cdot_\delta$

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(-v_\varepsilon c_\varepsilon + D_m \nabla c_\varepsilon) \cdot \nu_\varepsilon - \varepsilon \alpha_\delta f_\delta(c_\varepsilon, \rho_\delta)(c_\varepsilon - \rho_\delta) &= 0, && x \in \Gamma_\varepsilon(t),\ t \in (0,T)
\end{aligned}
$$

Stokes equation for advective velocity v_ε and pressure p_ε

$$
\begin{aligned}
\varepsilon^2 \mu \Delta v_\varepsilon - \nabla p_\varepsilon &= 0, && x \in \Omega_\varepsilon(t), && t \in (0,T),\\
\nabla \cdot v_\varepsilon &= 0, && x \in \Omega_\varepsilon(t), && t \in (0,T),\\
v_\varepsilon &= \varepsilon \alpha_\delta f_\delta(c_\varepsilon, \rho_\delta) \nu_\varepsilon, && x \in \Gamma_\varepsilon(t), && t \in (0,T)
\end{aligned}
$$

Upscaling via two-scale asymptotic expansion in level-set framework [van Noorden]

$$P_\varepsilon : \mathcal{L}_\varepsilon \varphi_\varepsilon = f_\varepsilon \qquad\qquad P_0 : \bar{\mathcal{L}} \bar{\varphi}_0 = \bar{f}_0$$

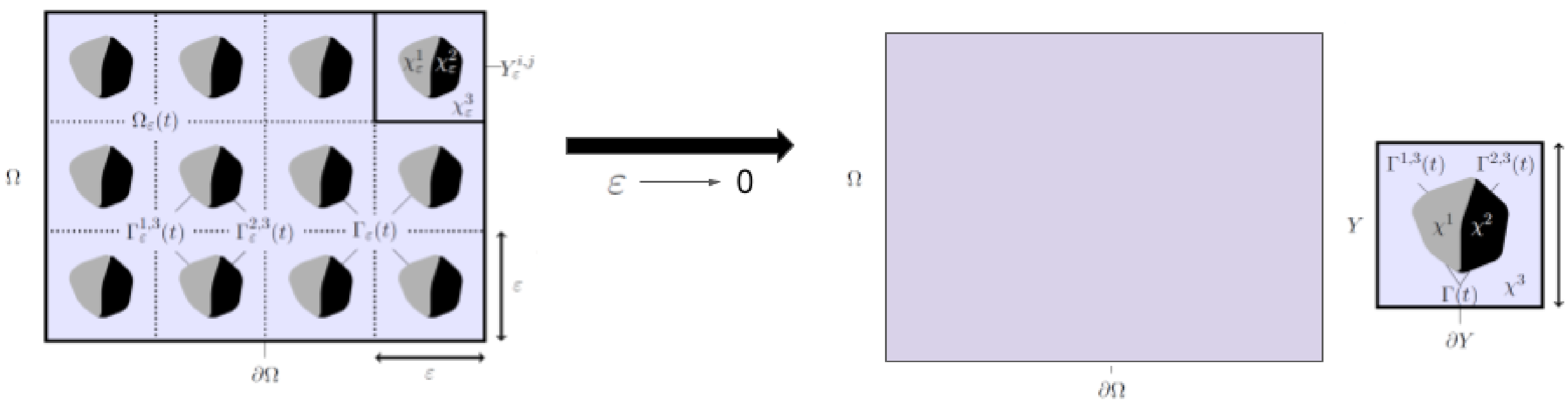


Figure: Upscaling concept. Left: idealized porous medium with scale parameter ε; Right: micro-macro model with unit cell.

Two-way coupled micro-macro model

Transport equation for the concentration c_0

$$\partial_t(\theta c_0) + \nabla_x \cdot (\bar{v}_0 c_0) - \nabla_x \cdot (D \nabla_x c_0) = -\sigma_{1,2} f_1(c_0) - \sigma_{1,3} f_2(c_0) \text{ in } \Omega \times (0,T)$$

with porosity θ, effective diffusion tensor D and specific surfaces $\sigma_{i,j}$.

Darcy equation for the averaged velocity field $\bar{v}_0$ and pressure p_0

$$\begin{aligned} \bar{v}_0 &= -\frac{K}{\mu} \nabla p_0, && \text{in } \Omega,\ t \in (0,T), \\ \nabla \cdot \bar{v}_0 &= -\sigma_{1,2}\alpha_1 f_1(c_0) - \sigma_{1,3}\alpha_2 f_2(c_0) && \text{in } \Omega,\ t \in (0,T). \end{aligned}$$

with permeability tensor K.

Level set equation for level set ϕ_0

$$\partial_t L_0 - f_\delta(x, t, c_0, \rho, y) |\nabla_y L_0| = 0 \qquad \text{in } Y \times \Omega \times (0,T)$$

Two-way coupled micro-macro model

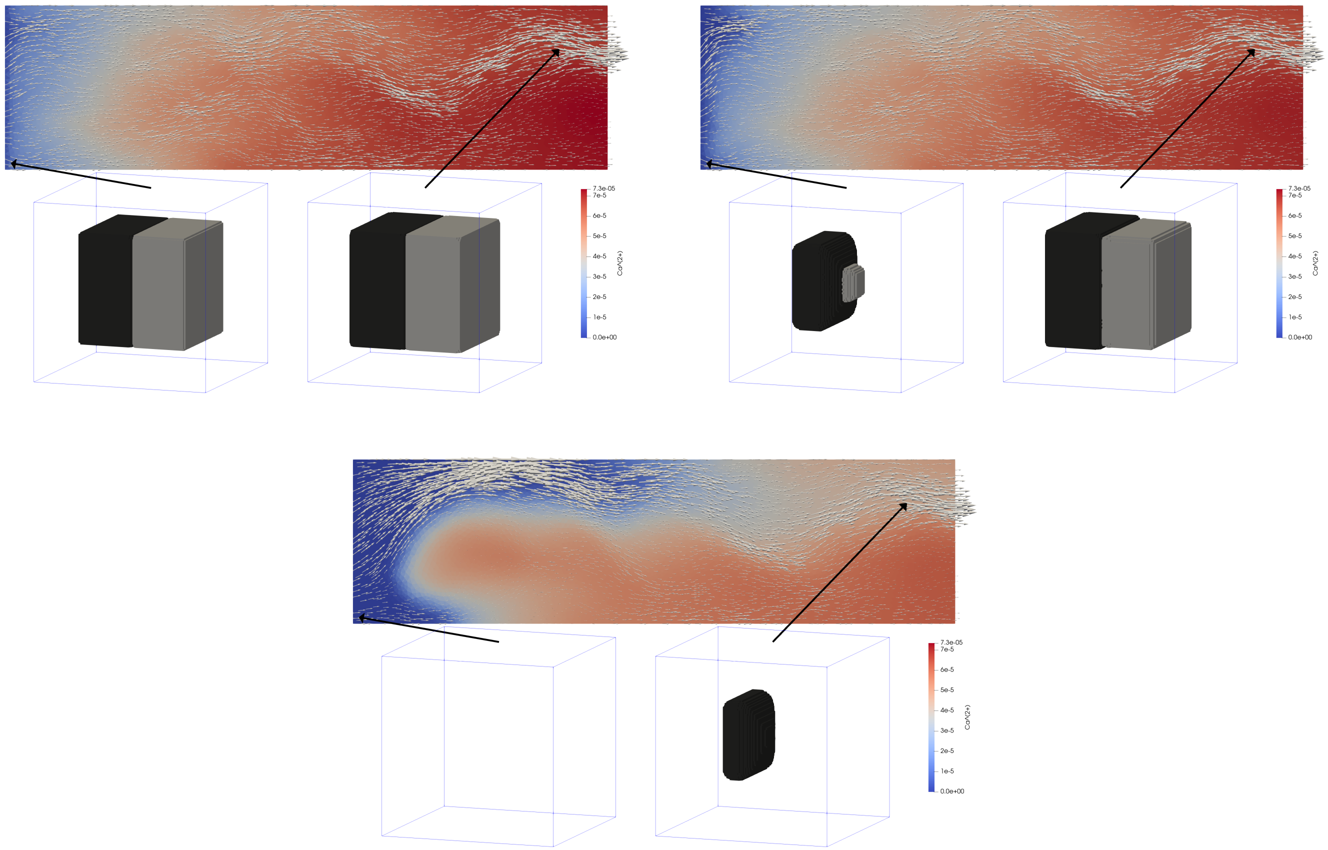
Cell problems in ζ_j for diffusion tensor

$$\begin{aligned} -\nabla_y \cdot (\nabla_y \zeta_j) &= 0 && y \in Y_{l,0}(t,x), \\ \nabla_y \zeta_j \cdot \nu_0 &= -e_j \cdot \nu_0 && y \in \Gamma_0(t,x), \\ \zeta_j \text{ periodic in } y, \quad \int_{Y_{l,0}(t,x)} \zeta_j \, dy &= 0. \end{aligned}$$

Cell problems in ω_j, π_j for permeability tensor

$$\begin{aligned} -\Delta_y \omega_j + \nabla_y \pi_j &= e_j && y \in Y_{l,0}(t,x), \\ \nabla_y \cdot \omega_j &= 0 && y \in Y_{l,0}(t,x), \\ \omega_j &= 0 && y \in \Gamma_0(t,x), \\ \omega_j, \pi_j \text{ periodic in } y, \quad \int_{Y_{l,0}(t,x)} \pi_j \, dy &= 0. \end{aligned}$$

Simulation scenario



Click for video

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Open position

Within the DFG funded Priority Program PP 2089 „Rhizosphere Spatiotemporal Organisation – a Key to Rhizosphere Functions" we offer a three year

PhD Position "Reactive Transport and Structure Formation in Porous Media"

in the section „Modelling and Numerics" at the Department of Mathematics, Friedrich-Alexander Universität Erlangen-Nürnberg/Germany.

Please send your application (cover letter, CV, an official listing of your grades, and contact details of a reference) electronically to prechtel@math.fau.de

Interpolation

$$h_\delta(x) = \begin{cases} \left[\frac{\text{dist}(x,\tilde{\chi}_\varepsilon^2(t))}{2\delta\varepsilon} + \frac{1}{2}\right] h_1(x) + \left[-\frac{\text{dist}(x,\tilde{\chi}_\varepsilon^2(t))}{2\delta\varepsilon} + \frac{1}{2}\right] h_2(x), \text{ if } 0 < \text{dist}(x, \tilde{\chi}_\varepsilon^2(t)) \le \delta\varepsilon \\ \left[-\frac{\text{dist}(x,\tilde{\chi}_\varepsilon^1(t))}{2\delta\varepsilon} + \frac{1}{2}\right] h_1(x) + \left[\frac{\text{dist}(x,\tilde{\chi}_\varepsilon^1(t))}{2\delta\varepsilon} + \frac{1}{2}\right] h_2(x), \text{ if } 0 < \text{dist}(x, \tilde{\chi}_\varepsilon^1(t)) \le \delta\varepsilon \\ h_1(x), \text{ if dist}(x, \tilde{\chi}_\varepsilon^2(t)) > \delta\varepsilon \\ h_2(x), \text{ if dist}(x, \tilde{\chi}_\varepsilon^1(t)) > \delta\varepsilon. \end{cases}$$

where

$$\tilde{\chi}_\varepsilon^i(t) := \left\{x \in \Omega : \text{dist}\left(x, \chi_\varepsilon^i(t)\right) < \text{dist}\left(x, \chi_\varepsilon^j(t)\right)\right\}, \quad j \neq i \in \{1, 2\}$$

Interpolation

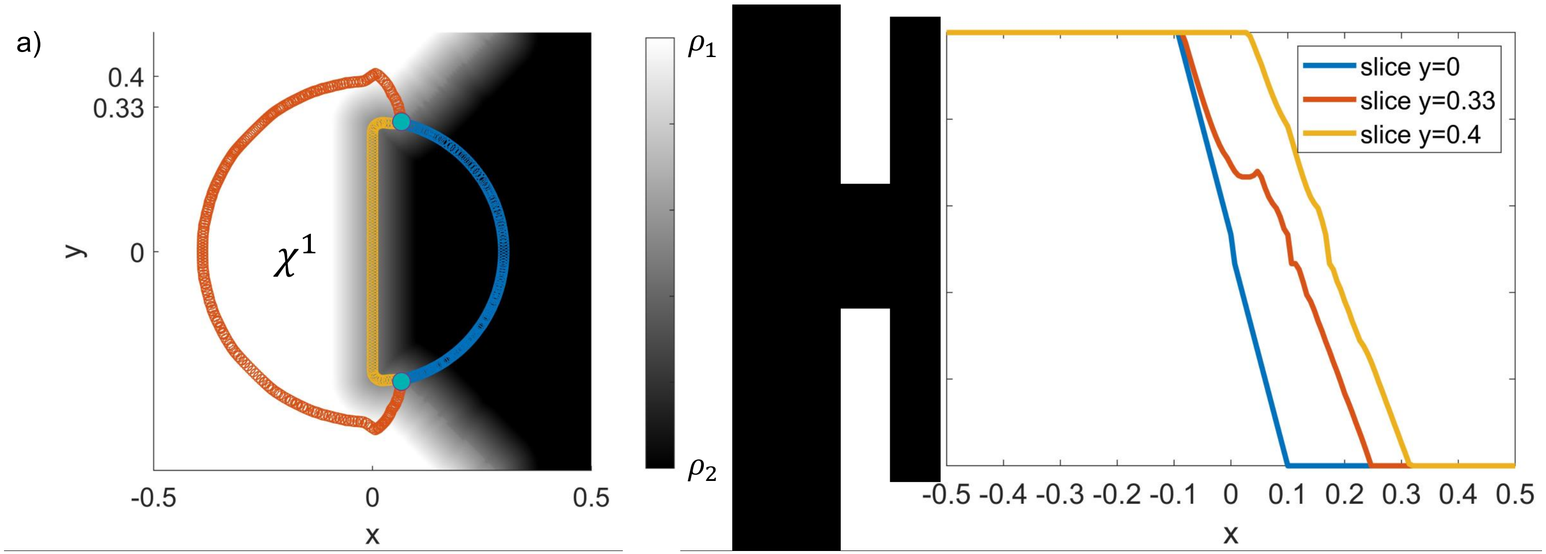

Figure: (a) Smoothing applied to mineral densities $\rho_1 > \rho_2$ being related to phases χ^1 and χ^2 for $\delta = 0.1$. The part of the fluid-solid interface $\Gamma^{1,3}$ is highlighted in red, $\Gamma^{2,3}$ in blue. Illustration (b) presents the values of ρ_δ as the interpolation between both mineral densities $\rho_1,\ \rho_2$ along different horizontal slices.