Discontinuous Galerkin discretization of phase-field models for pore-scale flows

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joint work with Lu Lin, Chen Liu, Christopher Thiel and Beatrice Rivière

SIAM GS21, Milan
June 24, 2021

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Introduction

We consider **at the pore-scale**:

- Immiscible components, e.g. oil and water.
- Effect of surfactants.
- Partially miscible components, e.g. methane and decane.

Diffuse-interface model:

- Based on thermodynamics.
- Assume a zone of phase-transition (opposed to sharp interfaces).
- Equations derived from a single energy functional.

Outline

- **Sur**factant loaded **C**ahn-**H**illiard (SurCH) model
- Key properties
- Numerical scheme
- Computational results
- Partially miscible two-phase flow (Lu Lin)
- Conclusion and future scope

SurCH

Unknowns:

- Order parameter for immiscible phases $c : \Omega \times [0, T] \mapsto [-1, 1]$.
- Surfactant volume fraction $s : \Omega \times [0, T] \mapsto [0, 1]$.

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Helmholtz free-energy formulation :

$$\mathcal{F}(c, s) = \int_\Omega (F_c + F_s + F_{s,c})$$

$$F_c = \Phi(c) + \frac{\mathrm{Cn}^2}{2}|\nabla c|^2 \qquad \text{(bulk phases)}$$

$$F_s = \alpha_2 \Psi(s), \qquad \text{(surfactant)}$$

$$F_{s,c} = \underbrace{-\alpha_3 s\Phi(c)}_{\substack{\text{adsorption}\\ \text{at}\\ \text{interface}}} + \underbrace{\alpha_4 s c^2}_{\substack{\text{solubility}\\ \text{in}\\ \text{bulk}}} \qquad \text{(interaction)}$$

$$\Phi(c) = \underbrace{\frac{1}{4}(1 - c^2)^2}_{\text{Ginzburg-Landau}}, \quad \Psi(s) = \underbrace{s\log(s) + (1 - s)\log(1 - s) + \log(2)}_{\text{Flory-Huggins}}$$

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Chemical potentials:

$$\mu_c = \frac{\delta \mathcal{F}}{\delta c}, \quad \mu_s = \frac{\delta \mathcal{F}}{\delta s}$$

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Minimization of free energy and conservation of mass:

$$\begin{aligned}
\partial_t c - \frac{1}{\mathrm{Pe}_c} \nabla \cdot (M_c \nabla \mu_c) + \nabla \cdot (c \boldsymbol{v}) &= 0, \\
\partial_t s - \frac{1}{\mathrm{Pe}_s} \nabla \cdot (M_s \nabla \mu_s) + \nabla \cdot (s \boldsymbol{v}) &= 0, \\
\mu_c - \Phi'(c) + \mathrm{Cn}^2 \Delta c + \alpha_3 s \Phi'(c) - 2\alpha_4 c s &= 0, \\
\mu_s - \alpha_2 \Psi'(s) + \alpha_3 \Phi(c) - \alpha_4 c^2 &= 0
\end{aligned}$$

where

$$\begin{aligned}
\text{Solenoidal velocity field} &: \boldsymbol{v} \\
\text{Peclet numbers} &: \mathrm{Pe}_c, \quad \mathrm{Pe}_s \\
\text{Mobility functions} &: M_c, \quad M_s = s(1-s)
\end{aligned}$$

SurCH: Properties

Conservation of mass: For a closed system, i.e., $\boldsymbol{v}\big|_{\partial\Omega} = \mathbf{0}$

$$\int_\Omega c(x,t)\mathrm{d}\Omega = \int_\Omega c_0(x)\mathrm{d}\Omega, \quad \int_\Omega s(x,t)\mathrm{d}\Omega = \int_\Omega s_0(x)\mathrm{d}\Omega.$$

Energy decay: For the non-advective system $\boldsymbol{v} \equiv \mathbf{0}$

$$\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t} = \int_\Omega \frac{\delta\mathcal{F}}{\delta c}\partial_t c + \int_\Omega \frac{\delta\mathcal{F}}{\delta s}\partial_t s \leqslant 0.$$

We aim to develop a scheme that preserves these properties.

SurCH: Properties

Choice of energy functional based on the work by Engblom et al. (2013):

- Model simplicity
- Stability
- Recovery of adsorption isotherms

Alternate formulations exist in literature: James et al. (2004); Teigen et al. (2011); Laradji et al. (1992); Komura et al. (1997); Sman et al. (2006); Liu et al. (2010); Zhu et al. (2018, 2019, 2020); ...

SurCH: Numerical scheme

- Ω discretized using conforming cuboidal elements of size h.
- Interior Penalty Discontinuous Galerkin (IPDG) in space to solve for c, s (directly) and μ_c, μ_s (indirectly).
- Semi-implicit in time with convex-concave splitting of $\Phi(c)$.
- $\boldsymbol{v}$ obtained via an a priori solve of the incompressible Navier-Stokes.

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Mass conservation: By construction.

Discrete energy decay: Define the discrete free-energy at $t = t^n$ as

$$\mathcal{F}_h^n = (\Phi(c_h^n), 1) + \frac{\mathrm{Cn}^2}{2} a_{\mathcal{D}}(c_h^n, c_h^n) + \alpha_2(\Psi(s_h^n), 1) - \alpha_3(\Phi(c_h^n), s_h^n) + \alpha_4((c_h^n)^2, s_h^n).$$

where

$$a_{\mathcal{D}}(.\ ,\ .) \rightarrow \text{ discrete diff. op.} \qquad (.\ ,\ .) \rightarrow \ L_2 \text{ inner prod.}$$

Assuming $\boldsymbol{v} \equiv \boldsymbol{0}$ and $s_h^n \geqslant 0$, we can prove

$$\mathcal{F}_h^{n+1} \leqslant \mathcal{F}_h^n \ \ \forall\ n \geqslant 1.$$

A discontinuous Galerkin method for a diffuse-interface model of immiscible two-phase flows with soluble surfactant; D. Ray, C. Liu, B. Riviere; (to appear in Comp. Geosci.)

Adsorption isotherms:

Consider a planar interface with notations $i \to$ interface, $b \to$ bulk. Assume

- Dilute solution regime, i.e., $s_b \ll 1$.
- c profile independent of s at equilibrium.

Then, at equilbrium

$$c(x) = \tanh\left(\frac{x - x_0}{\sqrt{2}\mathrm{Cn}}\right), \quad x_0 = 0.5$$

$$s(x) = \frac{s_b}{s_b + s_q(x)}, \quad s_q(x) = \exp\left[-\frac{1}{\alpha_2}\left(\alpha_3\Phi(c(x)) + \alpha_4(1 - c(x)^2)\right)\right]$$

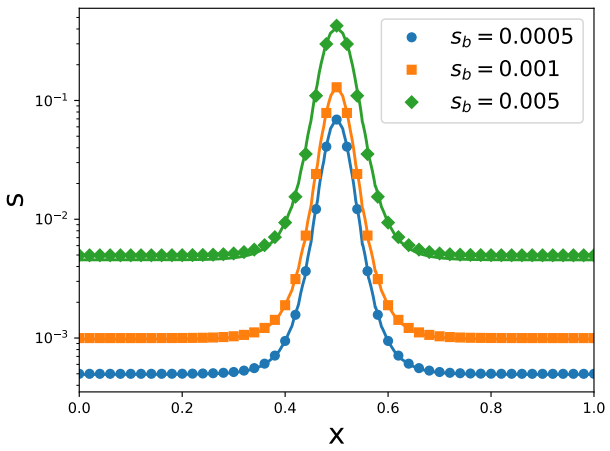
Specializing to the interface ($c_i = 0$)

$$\underbrace{s_i = \frac{s_b}{s_b + s_{q,i}}}_{\text{Langmuir isotherm}}, \quad \underbrace{s_{q,i} = \exp\left[-\frac{1}{\alpha_2}\left(\frac{\alpha_3}{4} + \alpha_4\right)\right]}_{\text{Langmuir adorption constant}}.$$

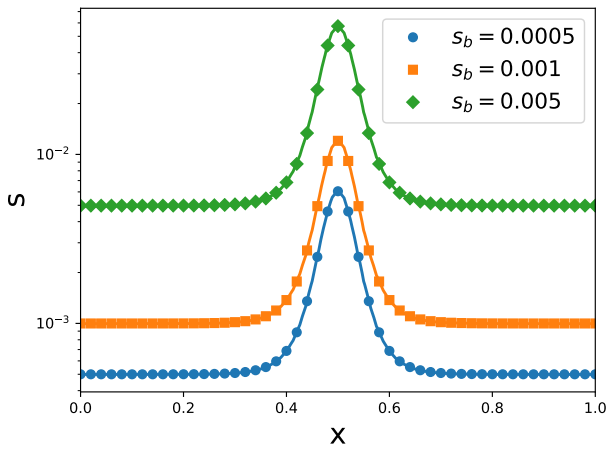
SurCH: Non-advective experiments

Adsorption isotherms:

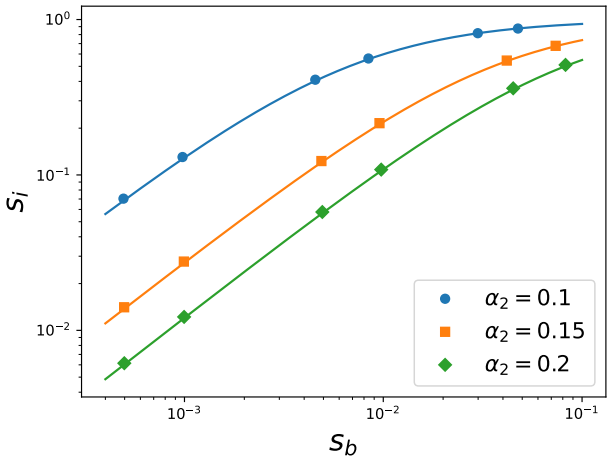
- Fixed: $\mathrm{Pe}_c = \mathrm{Pe}_s = 1.0$, $\alpha_3 = 1.0$, $\alpha_4 = 0.25$, $h = 1/80$, $\mathrm{Cn} = 4h$.
- Initial shifted profile $s(x) = \frac{s_b}{s_b + s_q(x-0.2)}$



$\alpha_2 = 0.1$



$\alpha_2 = 0.2$



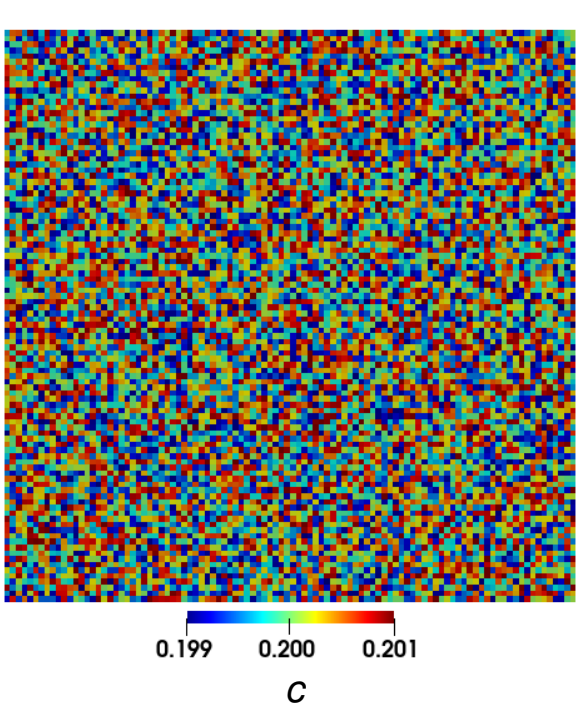
Langmuir isotherms

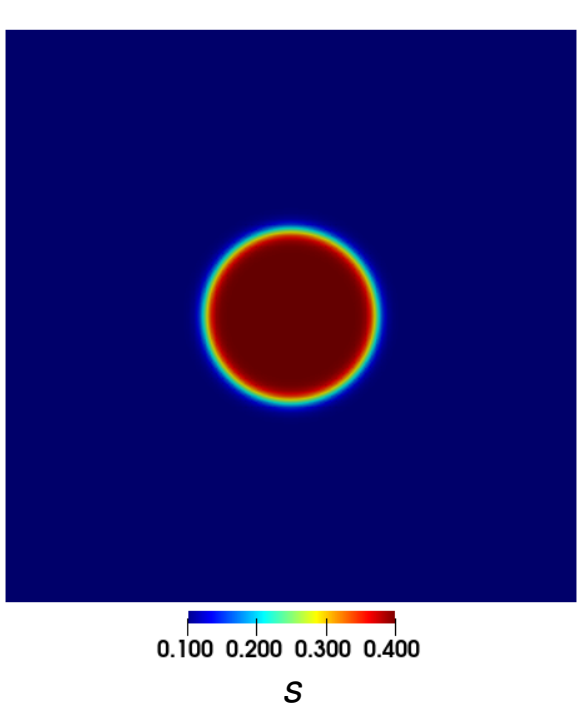
Numerical Analytical

Spinal-drop interaction:

$$c^0(x,y)\big|_{E_k} = 0.2 + 0.001\omega_k, \quad \omega_k \in \text{rand}([-1,1]),$$

$$s^0(x,y) = \frac{1}{2}\left(0.5 - 0.3\tanh\left(\frac{r_x - 0.15}{\sqrt{2}\text{Cn}}\right)\right), \quad r_x = \sqrt{(x-0.5)^2 + (y-0.5)^2}$$





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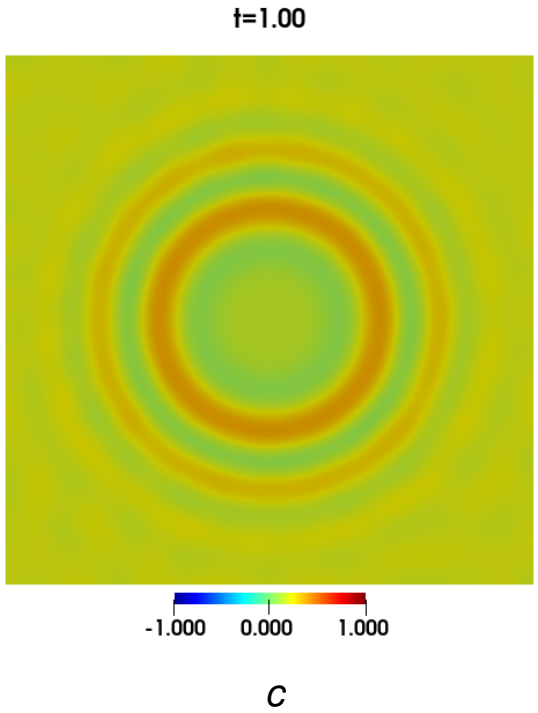
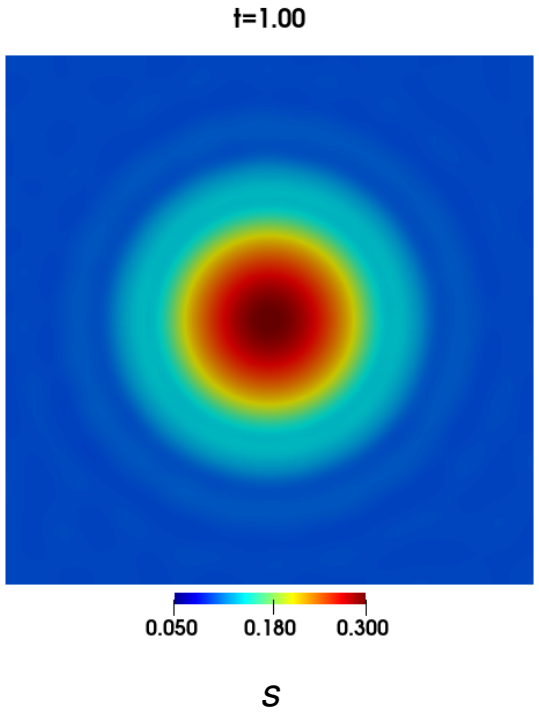


c



s

SurCH: Non-advective experiments

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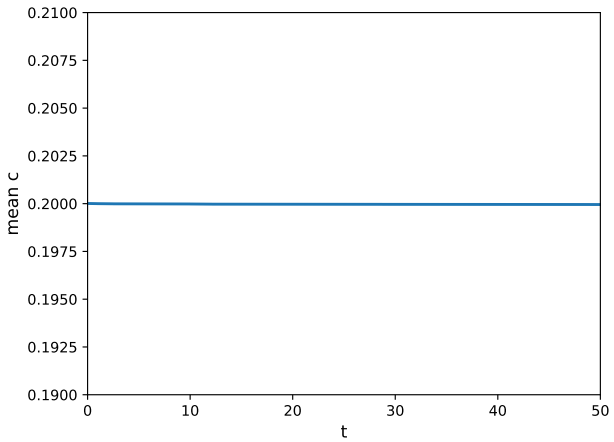
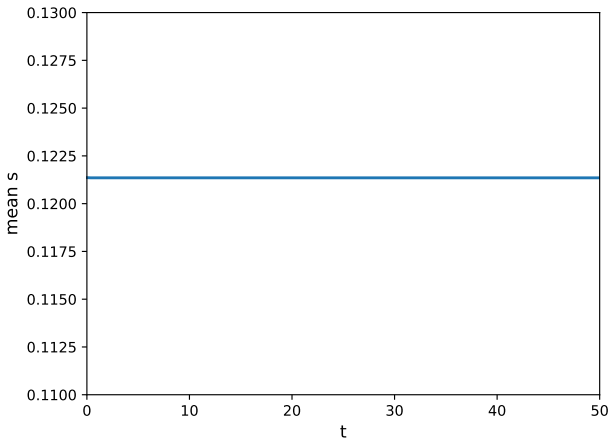
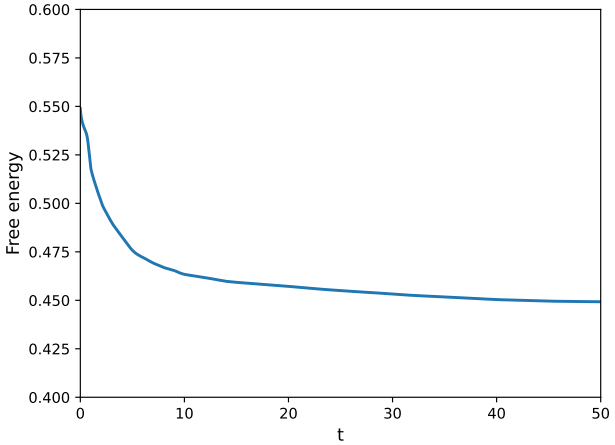


Conservation of c



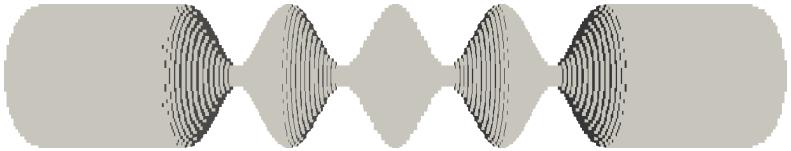
Conservation of s

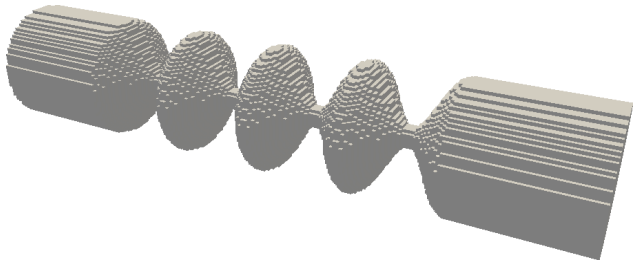


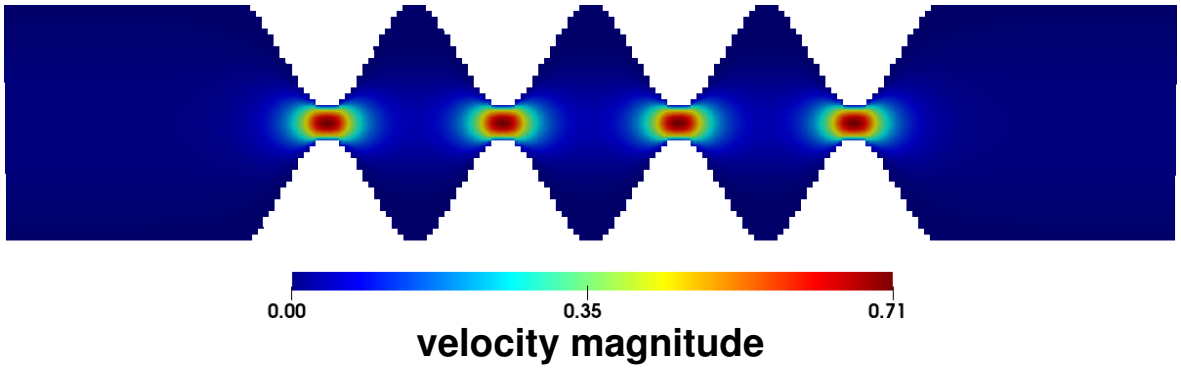
Energy decay

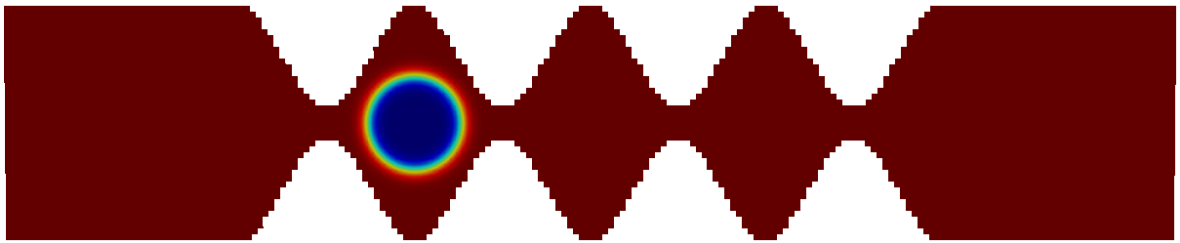
SurCH: Trapped oil drop

- **Domain:** $h = 1/200$, $r_{pipe} = 0.1$, $r_{throat} = 0.015$.





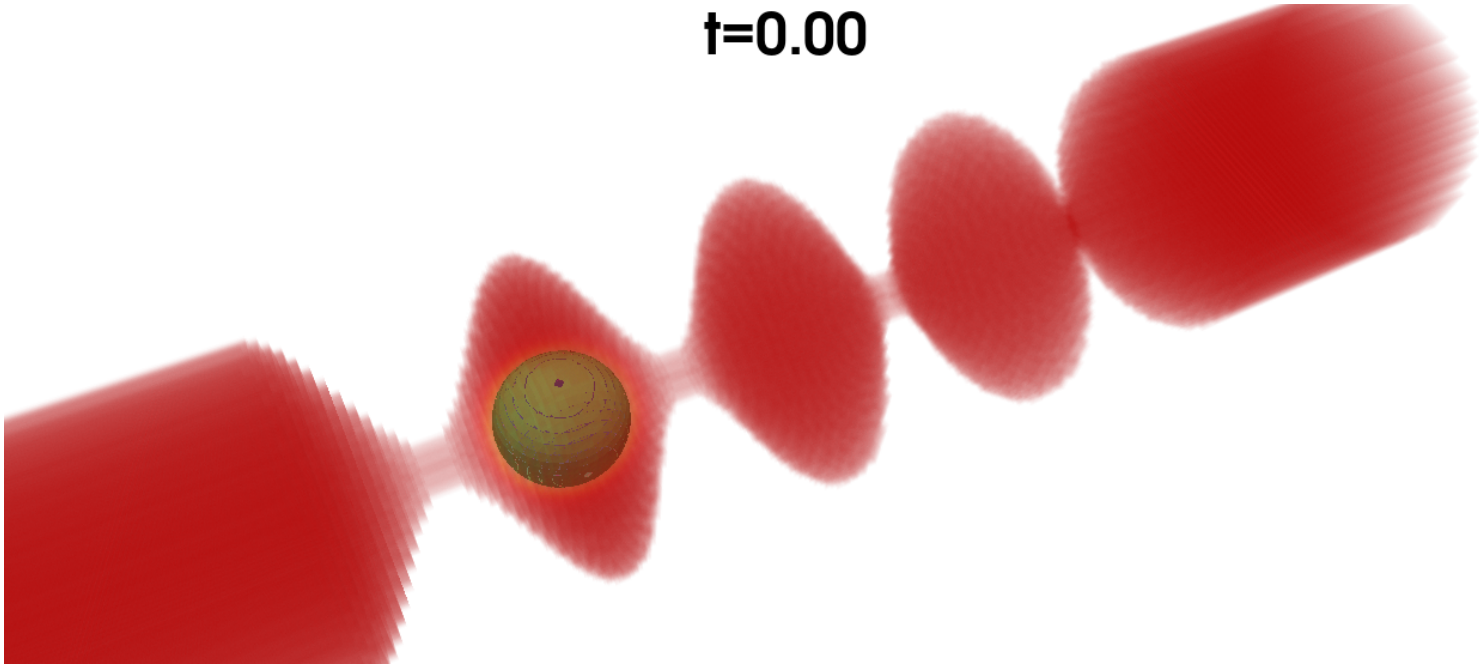




Initial c

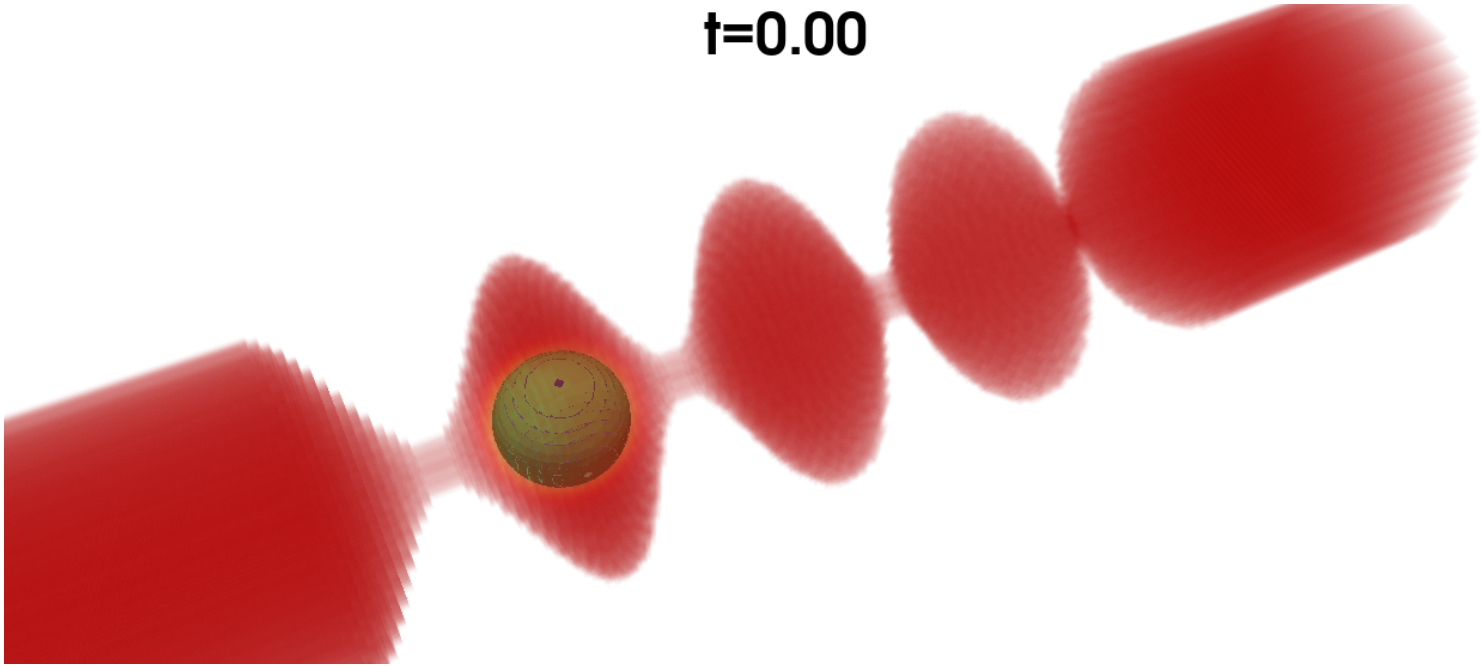
SurCH: Trapped oil drop

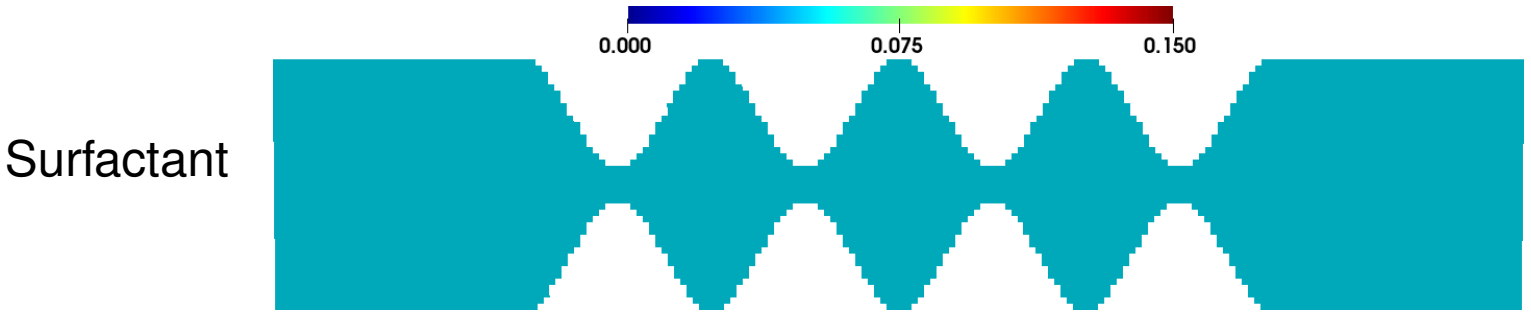
In the absence of surfactant



SurCH: Trapped oil drop

Flood with constant surfactant $s^0 = 0.05$.





SurCH: Trapped oil drop

Spontaneous shrinkage of drops [Yue et al., 2007]:
Drops in the Cahn-Hilliard framework will shrink and disappear if

$$r < r_c = \left(\frac{2^{1/6}}{3\pi} V\mathrm{Cn} \right)^{1/4} \approx 0.0923$$

where

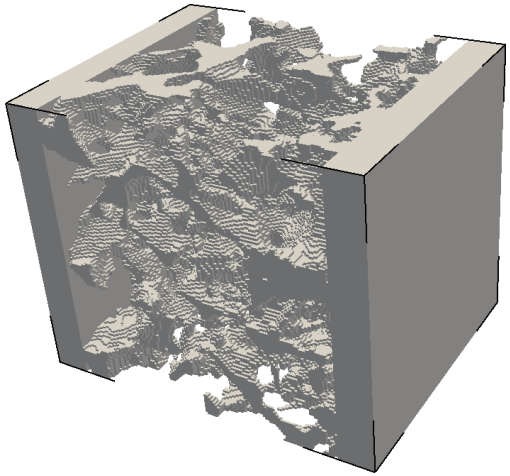
$$V \approx 0.1218 \quad \text{pore volume}, \quad \mathrm{Cn} = 5 \times 10^{-3}$$

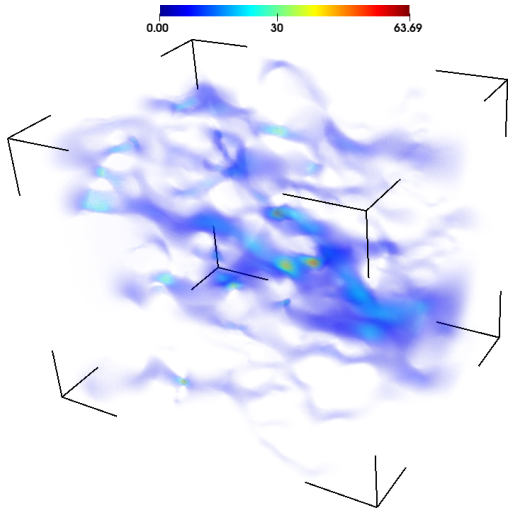
For our experiment $r = 0.04$.

SurCH: Flow through Berea sandstone (h=1/160)

- Pore space initially saturated with phase $c = -1$ and $s_0 = 10^{-3}$.
- Constant injection of second phase $c = 1$ and $s = 0.2$ at $x = 0$.

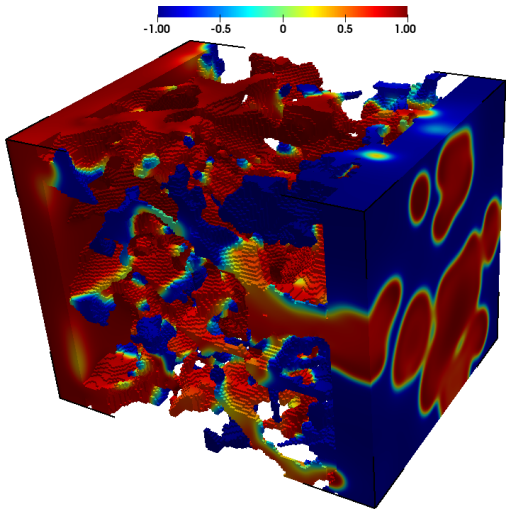
rock (gray)

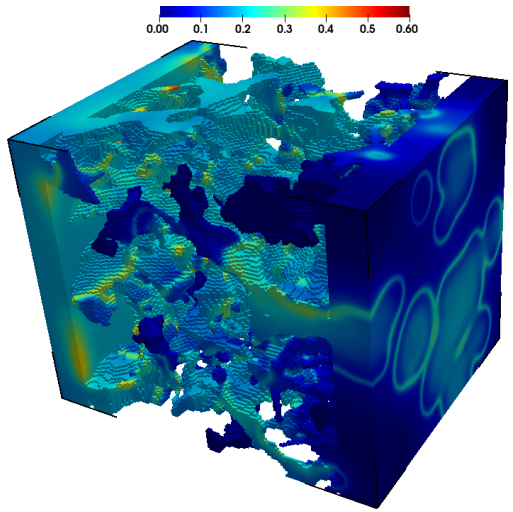




velocity field

c at $t = 1$

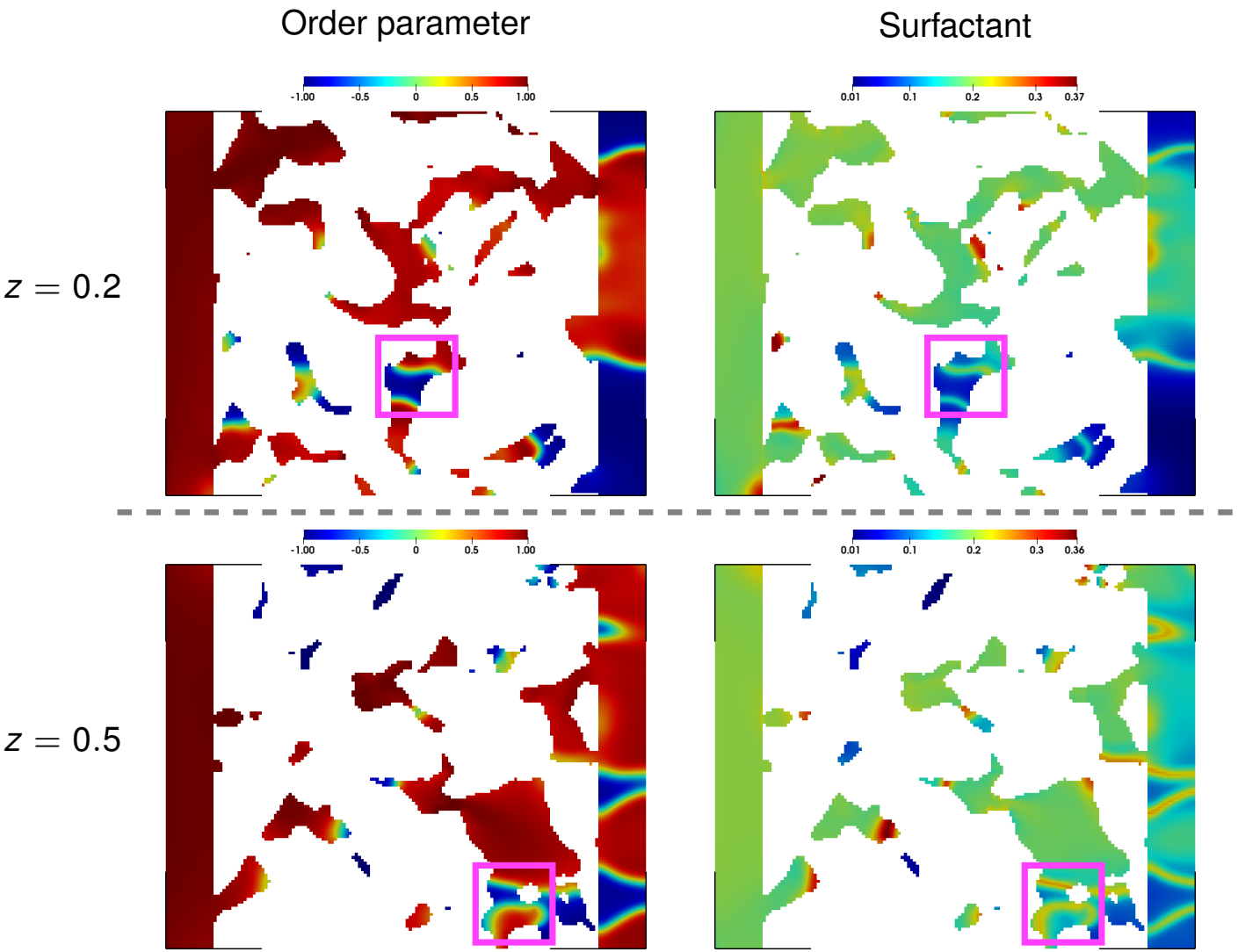




s at $t = 1$

SurCH: Flow through Berea sandstone (h=1/160)

2D slices parallel to flow



Partially miscible model

Two components (for instance methane and decane), with molar density $n_{1,2}$ and molar mass $\mathcal{M}_{1,2}$

$$\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \mathbf{v} - M_i \nabla \mu_i) = 0, \quad 1 \leqslant i \leqslant 2,$$

$$\mu_i = \frac{\partial \Psi}{\partial n_i} - \sum_{j=1}^{s} c_{ij} \Delta n_j, \quad 1 \leqslant i \leqslant 2,$$

$$\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\mathbf{v} \otimes (\rho \mathbf{v} - \underbrace{\sum_{j=1}^{2} \mathcal{M}_j M_j \nabla \mu_j}_{\text{coupling term}})) - \nabla \cdot \boldsymbol{\tau} = - \sum_{j=1}^{2} n_j \nabla \mu_j,$$

with

$$\boldsymbol{\tau} = 2G\boldsymbol{\epsilon}(\mathbf{v}) + (K - \frac{2}{3}G)(\nabla \cdot \mathbf{v})\mathbf{I}, \quad \boldsymbol{\epsilon}(\mathbf{v}) = \frac{1}{2}(\nabla \mathbf{v} + (\nabla \mathbf{v})^T), \quad \rho = \sum_{j=1}^{s} \mathcal{M}_j n_j.$$

Ψ : derived from Peng-Robinson EOS

Partially miscible model: Numerical scheme

- IPDG in space: unknowns are discontinuous piecewise linears: $n_{1h}, n_{2h}, \mathbf{v}_h$.
- Semi-implicit in time with convex-concave splitting for Ψ.
- Mass balance equations and momentum equations solved iteratively.
- Discrete total energy

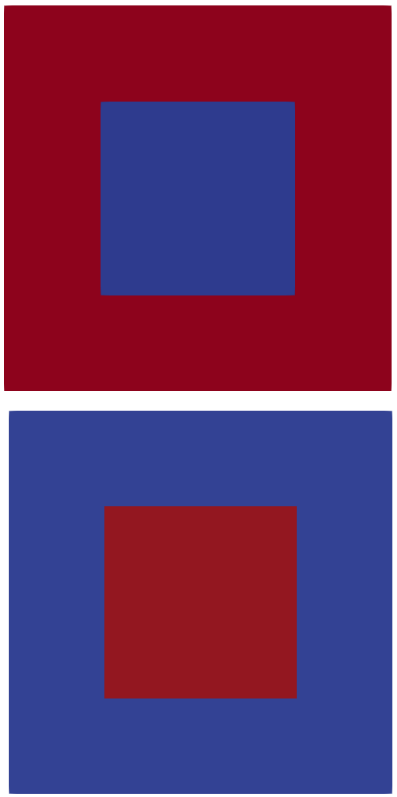
$$\mathcal{E}^k_{\mathrm{tot},h} = (\Psi(n^k_{1h}, n^k_{2h}), 1) + \frac{\mathrm{Cn}^2}{2} \sum_{i,j=1}^{2} c_{ij} a_{\mathcal{D}}(n^k_{ih}, n^k_{jh}) + \frac{\mathrm{Re}\,\mathrm{Ca}\,\mathrm{Cn}}{2}(\rho^k, \mathbf{v}^k_h \cdot \mathbf{v}^k_h).$$

We can prove (fully-implicit scheme):

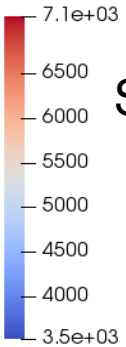
$$\mathcal{E}^k_{\mathrm{tot},h} \leqslant \mathcal{E}^{k-1}_{\mathrm{tot},h}, \quad \forall k \geqslant 1.$$

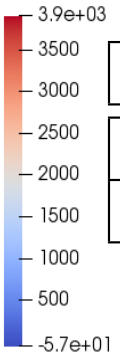
Partially miscible model: Droplet scenario

Simulate the dynamical evolution of a square liquid droplet in the center of a square domain.



t = 0





Setup:

- Two components: methane (n_1), decane (n_2)
- temperature: 320K
- initial molar density: mol/m^3

	inner phase	outer phase
n_1	3513.2	7133.9
n_2	3814.6	26.5

Partially miscible model: Droplet scenario

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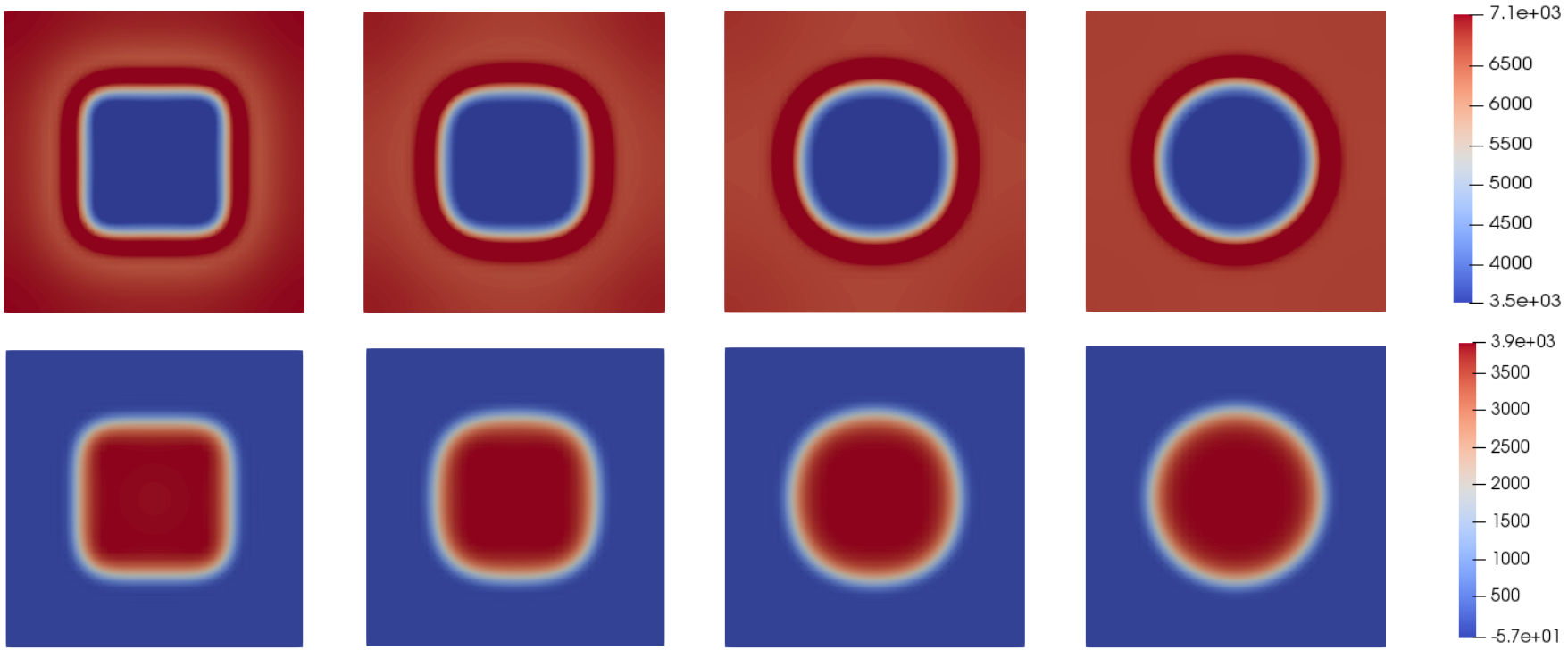

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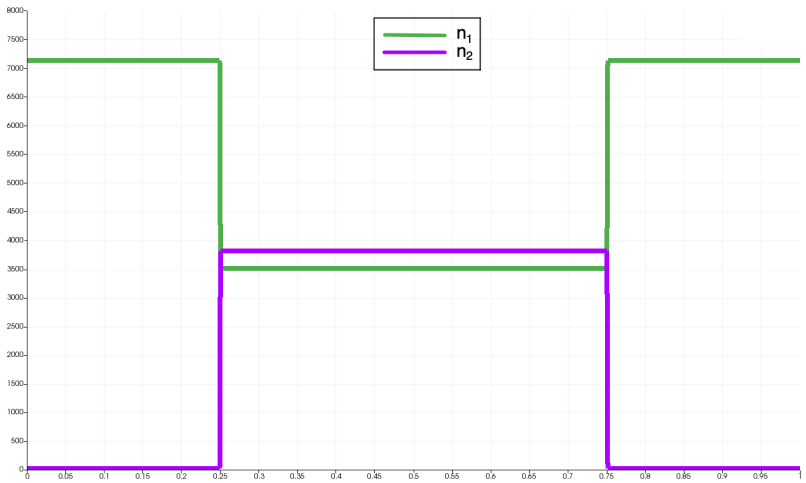
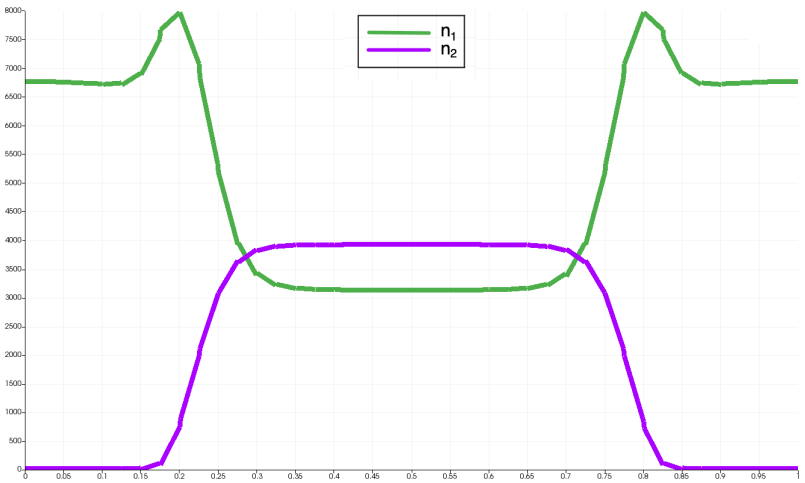


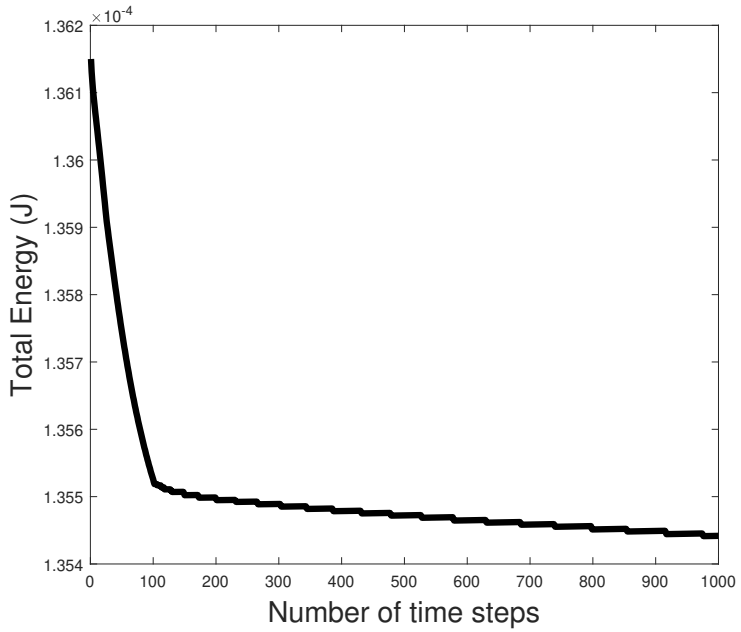
t = 0



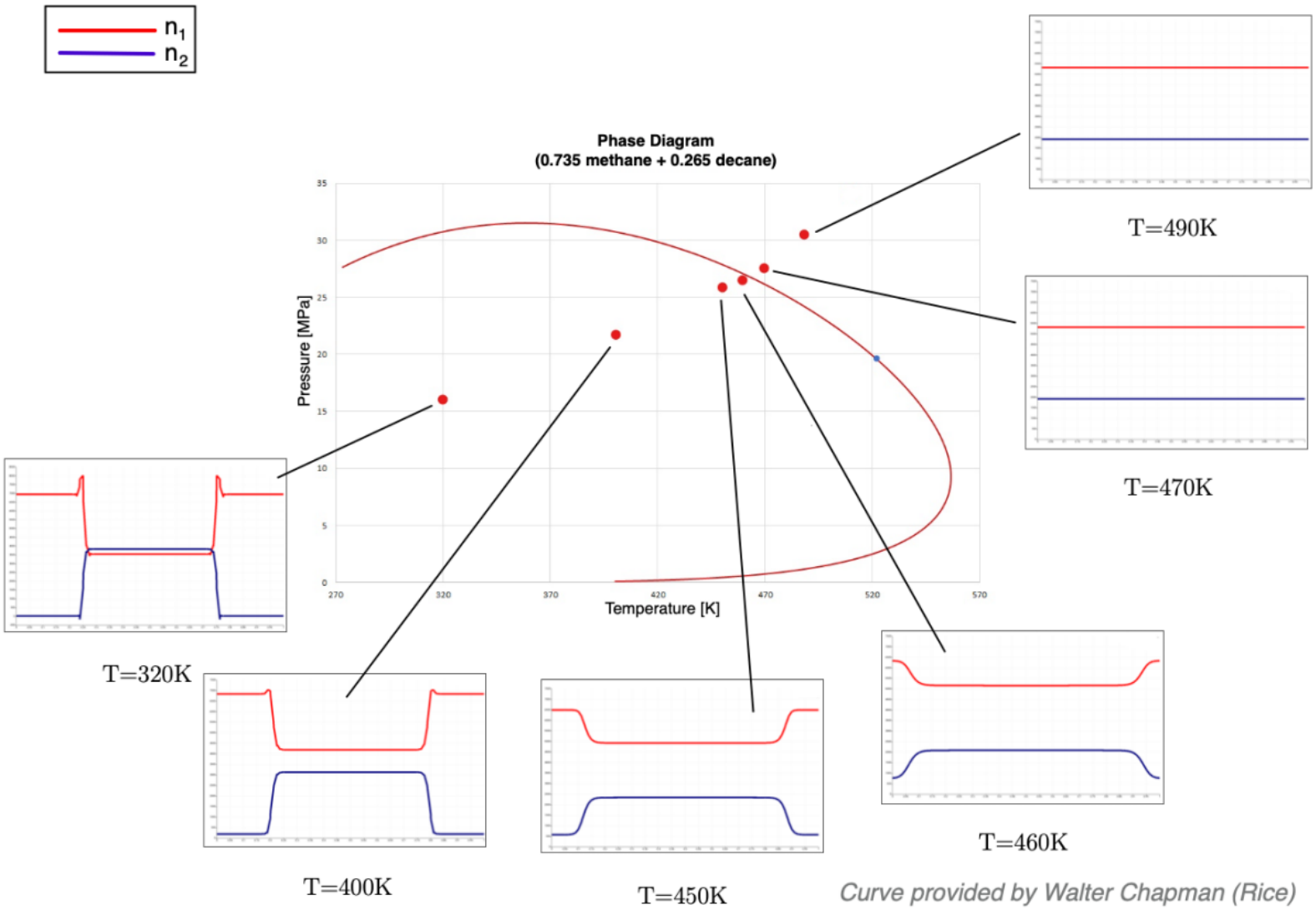
equilibrium

Partially miscible model: Droplet scenario

Simulate the dynamical evolution of a square liquid droplet in the center of a square domain.



Partially miscible model: Equilibrium composition



Curve provided by Walter Chapman (Rice)

Conclusion

- Developed an IPDG scheme for the SurCH model
  - Recovers (Langmuir) adsorption isotherms.
  - Conservative and energy stable.
  - Captures surfactant dynamics.
- Developed an IPDG scheme for partially miscible model
  - Captures expected equilibrium beviour.
  - Energy stable (empirically).

Conclusion

- Developed an IPDG scheme for the SurCH model
  - Recovers (Langmuir) adsorption isotherms.
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Future directions:

- Two-way coupling for SurCH.
- Include a wettability model.
- Use flux and slope limiter to control bulk-shift and spurious oscillations.
- Higher-order time-marching strategy ensuring energy decay.

Acknowledgments

- Dr. Steffen Berg for useful discussions on surfactant models.
- Shell-Rice collaboration.
- National Science Foundation.

Questions?

SurCH: boundary conditions

We consider the following boundary conditions

$$
\begin{aligned}
c &= c_{\text{in}}, \quad \text{on } \Gamma^{\text{in}} \times (0, T), \\
s &= s_{\text{in}}, \quad \text{on } \Gamma^{\text{in}} \times (0, T), \\
\nabla c \cdot \boldsymbol{n} &= 0 \quad \text{on } (\Gamma^{\text{wall}} \cup \Gamma^{\text{out}}) \times (0, T), \\
M_c \nabla \mu_c \cdot \boldsymbol{n} &= 0 \quad \text{on } \partial\Omega \times (0, T), \\
M_s \nabla \mu_s \cdot \boldsymbol{n} &= 0 \quad \text{on } \partial\Omega \times (0, T),
\end{aligned}
$$

where $c_{\text{in}} : \Gamma^{\text{in}} \times (0, T) \mapsto [-1, 1]$ and $s_{\text{in}} : \Gamma^{\text{in}} \times (0, T) \mapsto [0, 1]$.

SurCH: Simulation parameters

$M_c = 1$

Spinodal-drop: $h = 1/100$, $\mathrm{Pe}_c = \mathrm{Pe}_s = 100$, $\alpha_2 = \alpha_3 = \alpha_4 = 1$, $\tau = 10^{-3}$, $\mathrm{Cn} = h$

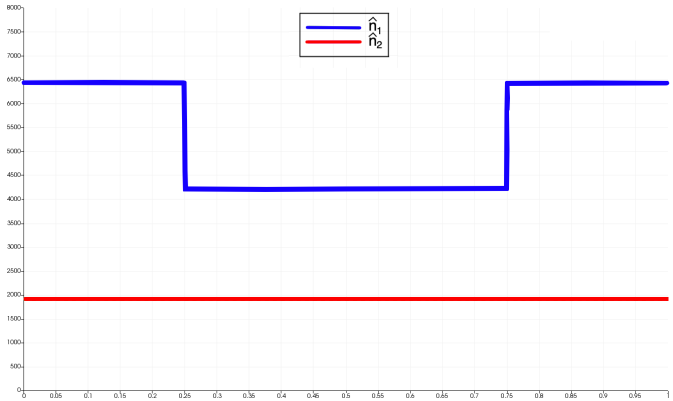
Trapped oil drop: $h = 1/200$, $\mathrm{Pe}_c = \mathrm{Pe}_s = 100$, $\alpha_2 = \alpha_3 = \alpha_4 = 1$, $\tau = 10^{-3}$, $\mathrm{Cn} = h$

Trapped oil drop: $h = 1/160$, $\mathrm{Pe}_c = \mathrm{Pe}_s = 100$, $\alpha_2 = \alpha_3 = \alpha_4 = 1$, $\tau = 5 \times 10^{-3}$, $\mathrm{Cn} = h$

Non-linear system solved using Newton's method (GMRES + Jacobi preconditioner)

Partially miscible model: Stability

Changing initial composition yields the same equilibrium state

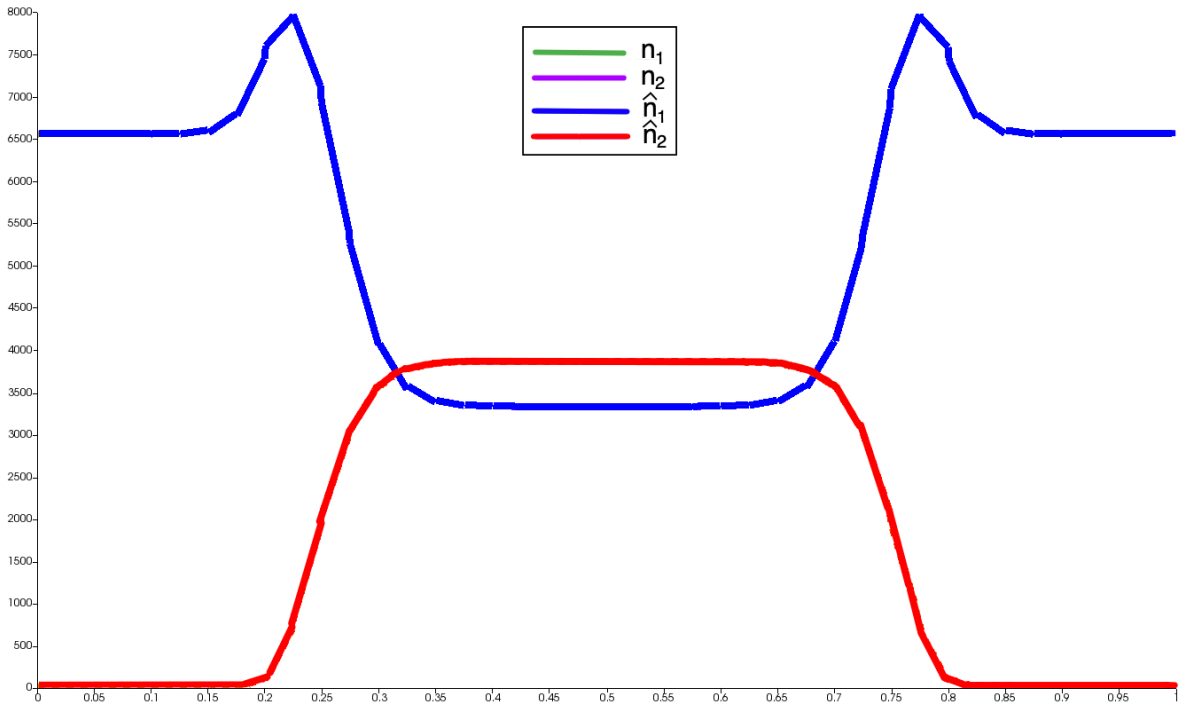


t = 0

Initial composition: perturb n_1 by 20% and take average for n_2

	inner phase	outer phase
$\hat{n}_1$	4215.84	6431.26
$\hat{n}_2$	1920.55	1920.55

Partially miscible model: Stability



equilibrium