

Analysis and Numerics of Viscoelastic Phase Separation

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collaboration with: **A. Brunk, B. Dünweg**



- Typical model: Cahn-Hilliard-Navier-Stokes system (Model H)

$$\begin{aligned}\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi &= \operatorname{div}(\phi^2(1-\phi^2)\nabla \mu) \\ \mu &= -\gamma \Delta \phi + f'(\phi) \\ \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} &= \operatorname{div}(\eta(\phi) D \mathbf{u}) - \nabla p + \nabla \phi \mu \\ \operatorname{div}(\mathbf{u}) &= 0\end{aligned}$$

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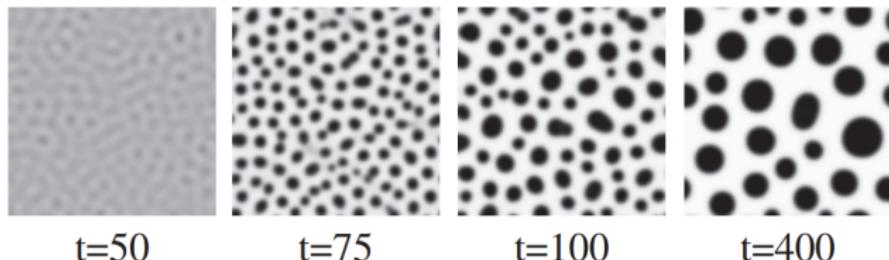


Figure: Simulation: Standard phase separation model

Phase separation of a polymeric fluid

Replacing one component by a polymer introduces new effects (transient gel)

¹ Tanaka: *Viscoelastic phase separation*, *J. Condens. Matter Phys.*, 2000

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viscoelastic relaxation in pattern formation ⇒

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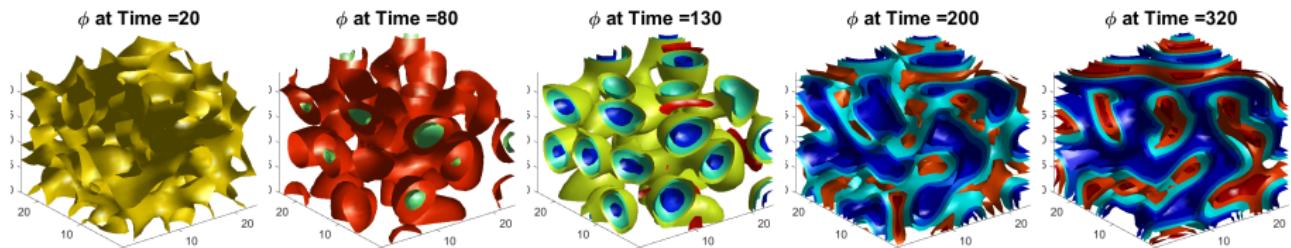
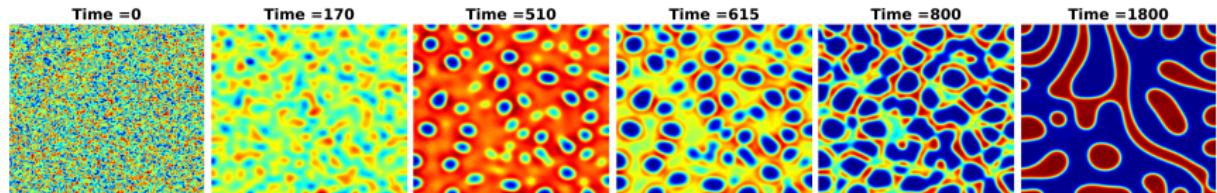
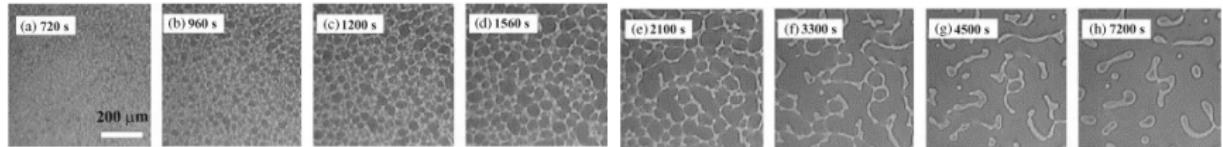
Phase separation of a polymeric fluid

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- Dynamic asymmetry of the components (slow and fast components)
- Relaxation effects for polymer and solvent on different timescales
viscoelastic relaxation in pattern formation ⇒
- Transient network structure of slow phase
⇒ Flow through a porous medium (polymer network)
- Tanaka¹ proposed a concept of viscoelastic phase separation

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Experiments(PS/PVME) and simulations



Top: Tanaka's real experiments, Mid: 2D simulation, Bottom: 3D simulations via variational methods.

Literature overview

- Elliott, Garcke ('96) ... CH with degenerate mobilities
- Ables ('09) ... CH-NS
- Abels, Depner, Garcke ('13) ... CH-NS with degenerate mobilities
- Abels, Garcke, Grün ('12) ... two-phase model, different densities
- Cancés et al. ('19) ... CH as constrained Wasserstein gradient flow
- Grün, Metzger ('16) ... micro-macro models two-phase, dilute polymers

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- Barrett, Boyaval ('09) ... existence, regularized Oldroyd-B
- Barrett, Suli ('12-'18) ... existence diffusive Oldroyd-B
- Lei, Masmoudi, Zhou ('05) ... blow-up criterion
- Chupin ('18) ... strong sols.
- Constantin, Kriegl ('12) ... global regularity in 2D
- Geissert et al. ('12) ... strong sols.
- Lu, Zhang ('18) ... relative energy
- Zhang, Fang ('12) ... global strong sol. in critical L^p spaces
- Bathory, Bulíček, Málek ('24) ... existence, NSF & Johnson-Segalman stress-diffusive viscoelastic model
- Bulíček, Málek, Průša, Suli ('21) ... incomp. heat-conducting stress-diffusive rate-type model
- Bulíček, Los, Málek ('25) ... 3D Giesekus models

Macro Model

- ϕ polymer volume fraction ($(1 - \phi)$ solvent volume fraction)
- q bulk stress related to polymer effects
- σ viscoelastic stress
- \mathbf{u} volume-averaged velocity of polymers and solvents

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Variational principle: minimizing the total energy

$$E = F(\phi) + \int \frac{1}{2} q^2 + \int \frac{1}{2} \text{Tr}(\sigma) + \int \frac{1}{2} |u|^2, \quad \frac{d}{dt} E \leq 0$$

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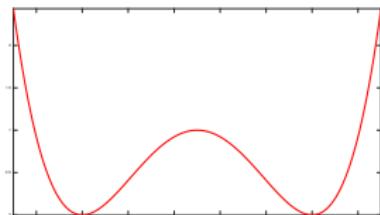
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- $F(\phi)$... free energy

$$F(\phi) = \int f(\phi) + \frac{\gamma}{2} |\nabla \phi|^2 dx$$



Viscoelastic phase separation I [Zhou, Zhang and E ('06)]

- ϕ polymer volume fraction ($(1 - \phi)$ solvent volume fraction)
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$$\begin{aligned}\partial_t \phi + \mathbf{u} \cdot \nabla \phi &= \operatorname{div} \left(\overbrace{\phi^2 (1 - \phi)^2}^{m(\phi)} \nabla \mu \right) - \operatorname{div} \left(\overbrace{\phi (1 - \phi)}^{n(\phi)} \nabla (A(\phi) q) \right) \\ \mu &= -c_0 \Delta \phi + f'(\phi) \\ \partial_t q + \mathbf{u} \cdot \nabla q &= -\frac{1}{\tau_b(\phi)} q + A(\phi) \Delta (A(\phi) q) - A(\phi) \operatorname{div} \left(\overbrace{\phi (1 - \phi)}^{n(\phi)} \nabla \mu \right) \\ \partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} &= \operatorname{div} (\eta(\phi) D \mathbf{u}) - \nabla p + \operatorname{div} \boldsymbol{\sigma} - \operatorname{div} (\gamma \nabla \phi \otimes \nabla \phi) \\ \operatorname{div} (\mathbf{u}) &= 0 \\ \partial_t \boldsymbol{\sigma} + (\mathbf{u} \cdot \nabla) \boldsymbol{\sigma} &= (\nabla \mathbf{u}) \boldsymbol{\sigma} + \boldsymbol{\sigma} (\nabla \mathbf{u})^\top - \frac{1}{\tau_s(\phi)} \boldsymbol{\sigma} + B(\phi) D \mathbf{u}\end{aligned}$$

$$E(\phi, q, \mathbf{u}, \boldsymbol{\sigma}) = \int \frac{\gamma}{2} |\nabla \phi|^2 + f(\phi) + \frac{1}{2} |q|^2 + \frac{1}{2} |\mathbf{u}|^2 + \frac{1}{2} \operatorname{tr}(\boldsymbol{\sigma}).$$

Viscoel. phase separation II [Brunk, ML (Nonlinearity '22)]

$$\begin{aligned}\partial_t \phi + \mathbf{u} \cdot \nabla \phi &= \operatorname{div}(m(\phi) \nabla \mu) - \operatorname{div}(n(\phi) \nabla (A(\phi)q)) \\ \mu &= -\gamma \Delta \phi + f'(\phi) \\ \partial_t q + \mathbf{u} \cdot \nabla q &= -\frac{1}{\tau(\phi)} q + A(\phi) \Delta (A(\phi)q) - A(\phi) \operatorname{div}(n(\phi) \nabla \mu) + \varepsilon_1 \Delta q \\ \partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} &= \operatorname{div}(\eta(\phi) D\mathbf{u}) - \nabla p + \operatorname{div} \operatorname{tr}(\mathbf{C}) \mathbf{C} - \operatorname{div}(\gamma \nabla \phi \otimes \nabla \phi) \\ \operatorname{div}(\mathbf{u}) &= 0 \\ \partial_t \mathbf{C} + (\mathbf{u} \cdot \nabla) \mathbf{C} &= (\nabla \mathbf{u}) \mathbf{C} + \mathbf{C} (\nabla \mathbf{u})^\top - h(\phi) \operatorname{tr}(\mathbf{C}) [\operatorname{tr}(\mathbf{C}) \mathbf{C} - \mathbf{I}] + \varepsilon_2 \Delta \mathbf{C}\end{aligned}$$

- viscoelastic stress tensor $\mathbf{T} = \operatorname{tr}(\mathbf{C}) \mathbf{C} - \mathbf{I}$

$$E(\phi, q, \mathbf{u}, \mathbf{C}) = \int_{\Omega} \frac{\gamma}{2} |\nabla \phi|^2 + f(\phi) + \frac{1}{2} |q|^2 + \frac{1}{2} |\mathbf{u}|^2 + \frac{1}{4} \operatorname{tr}(\mathbf{T}) - 2 \ln \operatorname{tr}(\mathbf{C})$$

$$E(t) + \int_0^t D(s) \, ds \leq E(0)$$

- additional energy functional (Lyapunov functional)

$$E = \int_{\Omega} \frac{\gamma}{2} |\nabla \phi|^2 + f(\phi) + \frac{1}{2} |q|^2 + \frac{1}{2} |\mathbf{u}|^2 + \frac{1}{4} |\mathbf{C}|^2 \, dx$$

with energy dissipation

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$$\begin{aligned} & E(t) + \int_0^t \int_{\Omega} \left(\sqrt{m(\phi)} \nabla \mu - \nabla(A(\phi)q) \right)^2 + \varepsilon_1 |\nabla q|^2 + \eta(\phi) |\mathbf{D}(\mathbf{u})|^2 \\ & + \int_0^t \int_{\Omega} \frac{q^2}{\tau(\phi)} + \frac{\varepsilon_2}{2} |\nabla \mathbf{C}|^2 + \frac{1}{2} h(\phi) \text{tr}(\mathbf{C})^2 |\mathbf{C}|^2 - \frac{1}{2} h(\phi) \text{tr}(\mathbf{C})^2 = E(0) \end{aligned}$$

Well-posedness

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- ① Existence of solutions
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Well-posedness

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- ① Existence of solutions —→ *weak solutions*
- ② Uniqueness of solution
- ③ Solution depends continuously on data

► Existence [Brunk, M.L. (Nonlinearity 2022)]

There exists at least one global weak dissipative solution, in *two space dimensions*, which satisfies the integrated energy inequality.

Existence/ regular & singular case

Regular case

- All parametric functions are continuous and positively bounded
- $A(s)$ is allowed to be zero somewhere
- mobility functions $m(s), n(s)$

$$0 < m_1 \leq m(s) = n(s) \leq 1,$$

- mixing potential $f(s)$ is polynomial (Ginzburg-Landau) potential,
e.g. $f(s) = (s - 1)^2 s^2$

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Singular case

- mobility functions $m(s), n(s) = 0$ if and only if $s \in \{0, 1\}$

$$m(s) = n(s)^2$$

- mixing potential $f(s)$ is logarithmic (Flory-Huggins) potential

Weak solutions

► Brunk, ML (Nonlinearity '22)

For given initial conditions

$$(\phi_0, q_0, \mathbf{u}_0, \mathbf{C}_0) \in \left[H^1(\Omega) \times L^2(\Omega) \times L_\sigma^2(\Omega) \times (L^2(\Omega))^{2 \times 2} \right]$$

there exists a global weak solution of the regular problem with

$$\begin{aligned} \phi &\in L^\infty(0, T; H^1(\Omega)) \cap L^2(0, T; H^2(\Omega)), & \frac{\partial \phi}{\partial t} &\in L^2(0, T; H^{-1}(\Omega)) \\ \mathbf{u} &\in L^\infty(0, T; L_\sigma^2(\Omega)) \cap L^2(0, T; H_{0,\sigma}^1(\Omega)), & \frac{\partial \mathbf{u}}{\partial t} &\in L^2(0, T; H_{0,\sigma}^{-1}(\Omega)) \\ \mathbf{C}, q &\in L^\infty(0, T; L^2(\Omega)) \cap L^2(0, T; H^1(\Omega)), & \frac{\partial q}{\partial t}, \frac{\partial \mathbf{C}}{\partial t} &\in L^{\frac{4}{3}}(0, T; H^{-1}(\Omega)) \\ \mu &\in L^2(0, T; H^1(\Omega)), \end{aligned}$$

which obey the energy inequality

Existence of global weak dissipative solutions

- ① Existence of solutions 2D ✓
- ② Main problem

$$\frac{1}{2} [\nabla \mathbf{u} \mathbf{C} + \mathbf{C} (\nabla \mathbf{u})^T] : \mathbf{C} \neq \text{tr}(\mathbf{C}) \mathbf{C} : \nabla \mathbf{u} \text{ in 3D}$$

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- ⑤ Existence, regularity & weak-strong uniqueness for the Peterlin model in 3D
... Brunk, M.L., Lu: Commun. Math. Sci. 2022
- ⑥ Extension to a reduced viscoelastic phase separation model in 3D
... Brunk: DCDS 2022

Relative energy

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Let $E(z)$ be a convex energy, then the relative energy is given by

$$\mathcal{E}(z|\hat{z}) := E(z) - E(\hat{z}) - \left\langle \frac{\delta E}{\delta z}(\hat{z}), z - \hat{z} \right\rangle$$

- for non-convex double-well potential add a **penalty term**
- f is **λ -convex** if $f(z) + \lambda|z|^2$ is convex for some $\lambda > 0$
- for $d = 2$

$$\begin{aligned}\mathcal{E}(z|\hat{z}) := & \int_{\Omega} \frac{\gamma}{2} |\nabla(\phi - \hat{\phi})|^2 + f(\phi) - f(\hat{\phi}) - f'(\hat{\phi})(\phi - \hat{\phi}) \\ & + \frac{\alpha}{2} |\phi - \hat{\phi}|^2 + \frac{1}{2} |q - \hat{q}|^2 + \frac{1}{2} |\mathbf{u} - \hat{\mathbf{u}}|^2 + \frac{1}{4} |\mathbf{C} - \hat{\mathbf{C}}|^2\end{aligned}$$

$$\alpha > \lambda := \max\{\gamma, \gamma - \min f''\}$$

Relative energy

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- ① Uniqueness of solution → *weak-strong uniqueness*
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► Weak-strong uniqueness [Brunk, ML (ZAMM 2022)]

Compare a weak solution z with a more regular (strong) solution \hat{z} starting from the same initial data

$$\mathcal{E}(z|\hat{z})(t) + \mathcal{D}(t) \leq c(t)\mathcal{E}(z|\hat{z})(0) = 0$$

$$\begin{aligned}\mathcal{D} = & \frac{1}{2} \int_0^t \int_{\Omega} |n(\phi) \nabla(\mu - \hat{\mu}) - \nabla(A(\phi)(q - \hat{q}))|^2 + \frac{1}{\tau(\phi)} |q - \hat{q}|^2 \\ & + \varepsilon_1 |\nabla(q - \hat{q})|^2 + \eta(\phi) |D\mathbf{v} - D\hat{\mathbf{v}}|^2 + \frac{\varepsilon_2}{2} |\nabla(\mathbf{C} - \hat{\mathbf{C}})|^2 \\ & + h(\phi) \Phi(\text{tr}(\mathbf{C})) \text{tr}(\mathbf{C}) |\mathbf{C} - \hat{\mathbf{C}}|^2 dx dt'\end{aligned}$$

→ $z = \hat{z}$ weak-strong uniqueness

Stability estimate

Compare a weak solution z with arbitrary functions \hat{z} :

$$\mathcal{E}(z|\hat{z})(t) + \mathcal{D}(t) \leq e^{c(t)} \mathcal{E}(z|\hat{z})(0) + C e^{c(t)} \int_0^t \sum_{i=1}^5 \|r_i\|_*^2.$$

- residuals r_i study parameter changes, asymptotic limits, **coarse-graining errors for a hierarchy of models (relative entropy)** and convergence of numerical schemes

Error estimates I

- rigorous error estimate for the Cahn-Hilliard equation through the relative energy:

Brunk, Egger, Habrich, ML: M²AN'23

$$\mathcal{E}(z|\hat{z}) := \int \frac{\gamma}{2} |\nabla(\phi - \hat{\phi})|^2 + f(\phi) - f(\hat{\phi}) - f'(\hat{\phi})(\phi - \hat{\phi}) + \frac{\alpha}{2} |\phi - \hat{\phi}|^2$$

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- periodic BC, second order conforming finite elements
- Crank-Nicolson-type in time
- Let (ϕ, μ) be a regular periodic weak solution with $\phi_0 \in H^3(\Omega)$ s.t.

$$\begin{aligned}\phi &\in H^2(0, T; H^1(\Omega)) \cap H^1(0, T; H^3(\Omega)), \\ \mu &\in H^2(0, T; H^1(\Omega)) \cap L^\infty(0, T; W^{1,3}(\Omega)),\end{aligned}$$

and let $(\phi_{h,\tau}, \mathbf{u}_{h,\tau})$ be a solution of FEM.

- Then

$$\max_{t^n} \|\phi_{h,\tau}(t^n) - \phi(t^n)\|_{H^1} + \|\bar{\mu}_{h,\tau} - \bar{\mu}\|_{L^2(0,T;H^1)} \leq C_T(h^2 + \tau^2)$$

Error estimates II

- error estimates for Navier-Stokes-Cahn-Hilliard system:
Brunk, Egger, Habrich, ML: M³AS 2023
- Taylor-Hood (P2/P1) finite elements for the velocity and pressure
- P2 finite elements for ϕ, μ
- two-, three-dimensional model, periodic BC

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Let $(\phi, \mu, \mathbf{u}, p)$ is a regular sol., s.t.

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Then

$$\begin{aligned}\|\phi_{h,\tau} - \phi\|_{L_t^\infty, H_x^1} + \|\bar{\mu}_{h,\tau} - \bar{\mu}\|_{L_t^2, H_x^1} + \\ \|\mathbf{u}_{h,\tau} - \mathbf{u}\|_{L_t^\infty, L_x^2} + \|\bar{\mathbf{u}}_{h,\tau} - \bar{\mathbf{u}}\|_{L_t^\infty, L_x^2} \leq C(T)(h^2 + \tau^2)\end{aligned}$$

$\bar{\mathbf{u}}$... p.w. constant projection in time on (t^n, t^{n+1})

Error estimates III

- error estimates for Cahn-Hilliard model with bulk stress q :
Brunk, Egger, Habrich, ML: ArXiv 2024
- P2 finite elements for ϕ, μ, q
- two-, three-dimensional model, periodic BC
 - Let (ϕ, μ, q) is a regular sol., s.t.

$$\phi \in H^2(0, T; H^1(\Omega)) \cap H^1(0, T; H^3(\Omega)),$$

$$\mu \in H^2(0, T; H^1(\Omega)) \cap L^\infty(0, T; W^{1,3}(\Omega)) \cap L^2(0, T; H^3(\Omega))$$

$$q \in H^2(0, T; H^1(\Omega)) \cap L^\infty(0, T; W^{1,3}(\Omega)) \cap L^2(0, T; H^3(\Omega))$$

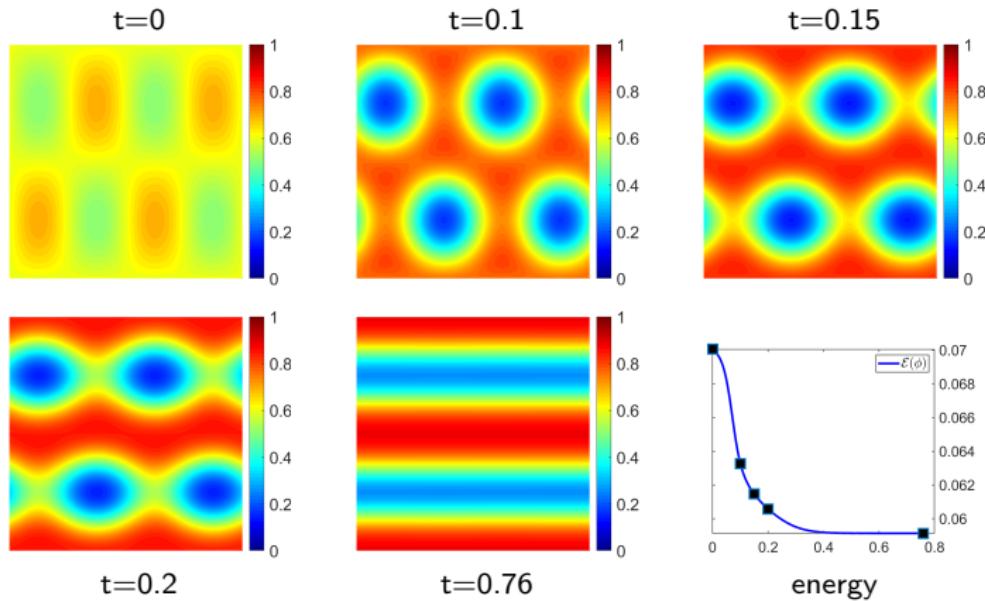
$$\begin{aligned} & \|\phi_{h,\tau} - \phi\|_{L_t^\infty, H_x^1} + \|q_{h,\tau} - q\|_{L_t^\infty, L_x^2} + \|\bar{\mu}_{h,\tau} - \bar{\mu}\|_{L_t^2, H_x^1} + \\ & \|\bar{q}_{h,\tau} - \bar{q}\|_{L_t^2, H_x^1} \leq C(T)(h^2 + \tau^2) \end{aligned}$$

\bar{q} ... p.w. constant projection in time on (t^n, t^{n+1})

Cahn-Hilliard eq.

- potential $f(\phi) = \frac{3}{2}(\phi \log(\phi) + (1 - \phi) \log(1 - \phi) + 3\phi(1 - \phi))$

$$\phi_0(x, y) = 0.1 \sin(4\pi x) \sin(2\pi y) + 0.6$$



Convergence rates

Table: Errors and convergence rates for the semi-discrete and fully-discrete approximations

k	e_h	eoc	$e_{h,\tau}$	eoc
0	$5.9075 \cdot 10^{-1}$	—	$5.9426 \cdot 10^{-1}$	—
1	$1.7016 \cdot 10^{-1}$	1.80	$1.7109 \cdot 10^{-1}$	1.79
2	$4.3761 \cdot 10^{-2}$	1.96	$4.4155 \cdot 10^{-2}$	1.95
3	$1.1038 \cdot 10^{-2}$	1.99	$1.1251 \cdot 10^{-2}$	1.97
4	$2.7658 \cdot 10^{-3}$	2.00	$3.3468 \cdot 10^{-3}$	1.74

Viscoelastic separation

- Cahn-Hilliard and q -equation

initial data:

$$\phi_0(x, y) = 0.25 \cos(2\pi x) \cos(2\pi y) + 0.5, \quad q_0(x, y) = 0.01 \sin(2\pi x) \sin(2\pi y).$$

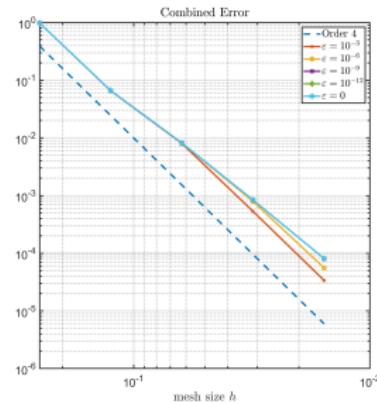
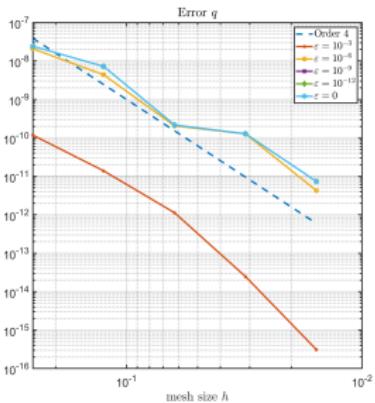
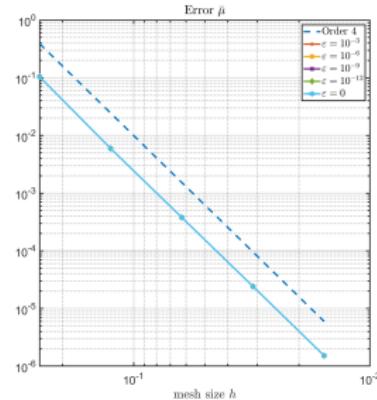
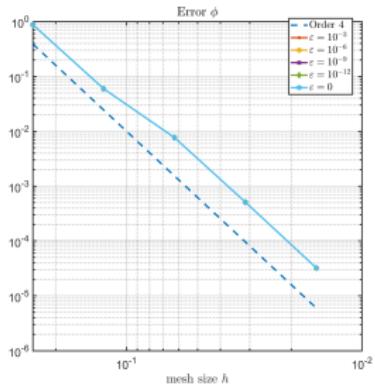
$$\gamma = 10^{-3}$$

$$M(\phi) = [\frac{4}{\sqrt{10}} \cdot \phi(1 - \phi)]^2 + \varepsilon, \quad f(\phi) = (\phi - 0.95)^2(\phi - 0.05)^2,$$

$$\tau_b(\phi) = 10^2(10\phi^2 + 10^{-4}), \text{ and}$$

$$A(\phi) = 5 \cdot 10^{-3} \cdot [1 + \tanh(5[\cot(\pi\phi^*) - \cot(\pi\phi)])]$$

with $\phi^* = \int_{\Omega} \phi_0$ denoting the total mass



Convergence rates for the errors in ϕ (top left), $\bar{\mu}$ (top right), q (middle left), \bar{q} (middle right) and the combined error (bottom) for different ε

Viscoelastic separation

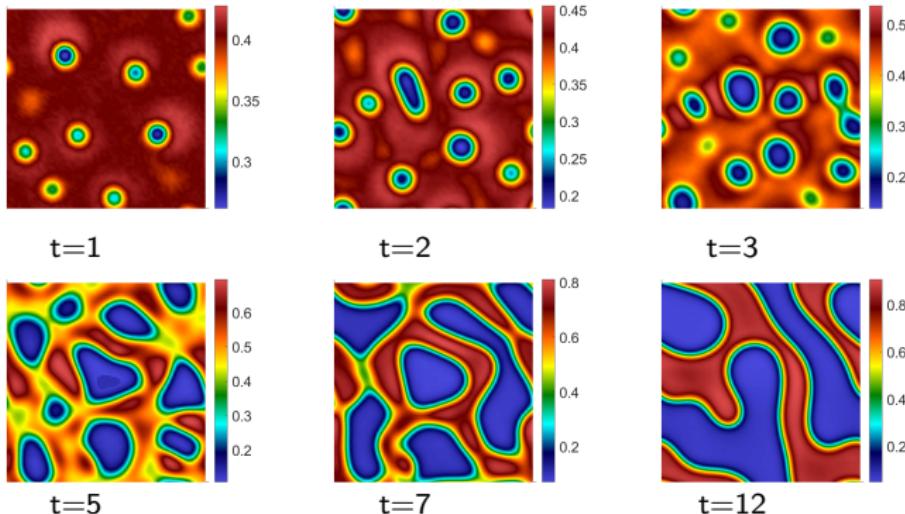
- Cahn-Hilliard and q -equation

initial data:

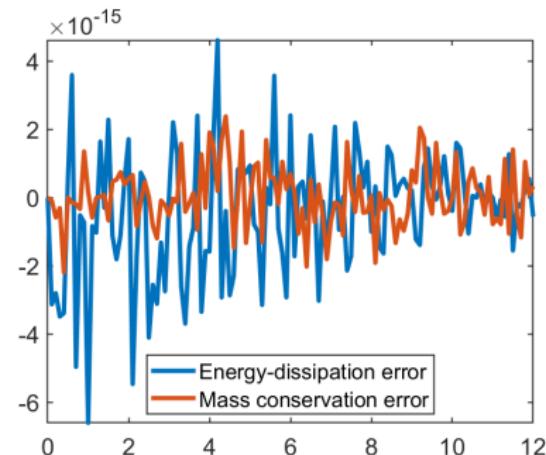
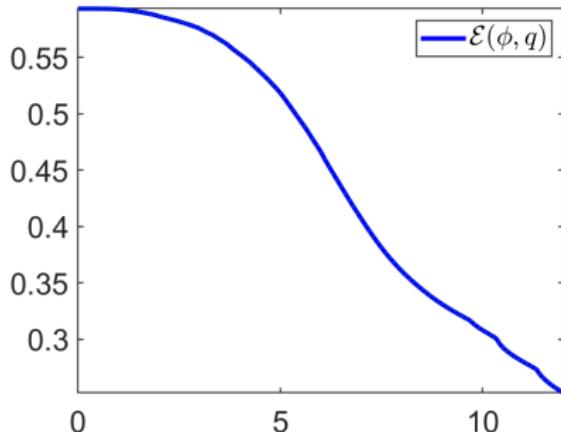
$$\phi_0(x, y) = 0.4 + \xi(x, y), \quad q_0 = 0, \quad \xi(x, y) \sim \mathcal{U}[-0.0025, 0.0025]$$

$$\gamma = \varepsilon = 10^{-3}, \quad f(\phi) = (\phi - 0.95)^2(\phi - 0.05)^2$$

$$A(\phi) = \frac{1}{2} [1 + \tanh(10[\cot(\pi\phi^*) - \cot(\pi\phi)])], \quad \phi^* = \int_{\Omega} \phi_0$$



Snapshots of the volume fraction ϕ with pure phases at $\phi = 0$ and $\phi = 1$

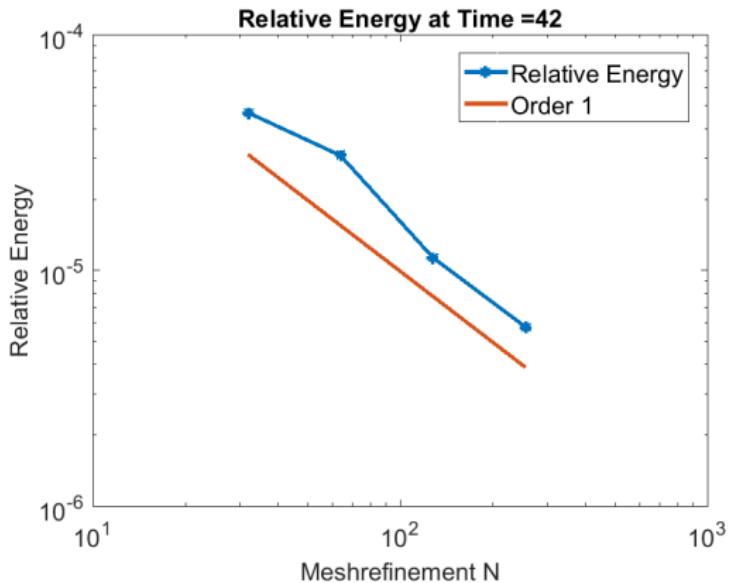


Temporal evolution of the energy (left) and the conservation and energy-dissipation error (right)

Full viscoelastic separation

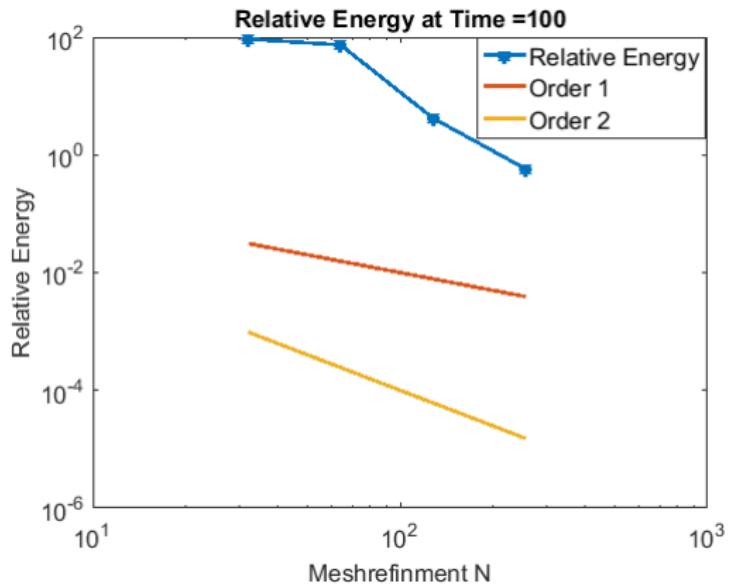
- characteristic FEM

- $\phi_0(x) = 0.4 + \xi(x)$, $q_0 = 0$, $\mathbf{u}_0 = \mathbf{0}$, $\mathbf{C}_0 = \frac{1}{\sqrt{2}}\mathbf{I}$
 $\xi(x)$ from $[-10^{-3}, 10^{-3}]$



Full viscoelastic separation

- $\phi_0(x) = 0.4 + 0.2 \sin\left(\frac{2\pi x}{128}\right) \sin\left(\frac{2\pi y}{128}\right)$, $q_0 = 0$, $\mathbf{u}_0 = \mathbf{0}$, $\mathbf{C}_0 = \frac{1}{\sqrt{2}}\mathbf{I}$



Peterlin viscoelastic system in 3D

$$\begin{aligned}\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} &= \operatorname{div}(\eta D\mathbf{u}) - \nabla p + \operatorname{div}(\mathbf{T}), \\ \frac{\partial \mathbf{C}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{C} &= (\nabla \mathbf{u}) \mathbf{C} + \mathbf{C} (\nabla \mathbf{u})^\top \\ &\quad + \Phi(\operatorname{tr}(\mathbf{C})) \mathbf{I} - \chi(\operatorname{tr}(\mathbf{C})) \mathbf{C} + \varepsilon \Delta \mathbf{C}, \\ \operatorname{div}(\mathbf{u}) &= 0, \quad \mathbf{T} = \operatorname{tr}(\mathbf{C}) \mathbf{C}.\end{aligned}$$

- $\Phi := \operatorname{tr}(\mathbf{C}) + a$ and $\chi := \operatorname{tr}(\mathbf{C})^2 + a|\operatorname{tr}(\mathbf{C})|$ for a given $a \geq 0$

Weak dissipative sol. in 3D / Peterlin model

Theorem (Brunk, ML, Lu (DCDS'22))

- *initial data* $(\mathbf{u}_0, \mathbf{C}_0) \in [L_\sigma^2 \times L^2(\Omega)]_{SPD}^{3 \times 3}$, $T > 0$.

There exists a global weak solution of the Peterlin system, s.t.

$$\mathbf{u} \in C_w([0, T]; L^2(\Omega)) \cap L^2(0, T; V) \cap C([0, T]; L^q(\Omega)) \cap W^{1, \frac{4}{3}}(0, T; V^*),$$

$$\mathbf{C} \in C_w([0, T]; L^2(\Omega)) \cap L^2(0, T; H^1(\Omega)) \cap L^4(\Omega_T)$$

$$\cap C([0, T]; L^q(\Omega)) \cap W^{1, \frac{4}{3}}(0, T; H^{-1}(\Omega)),$$

$$\chi(\text{tr}(\mathbf{C}))\mathbf{C} \in L^{\frac{4}{3}}(\Omega_T), \quad \Phi(\text{tr}(\mathbf{C})) \in L^2(\Omega_T), \quad \text{for any } 1 \leq q < 2$$

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$$\cap C([0, T]; L^q(\Omega)) \cap W^{1, \frac{4}{3}}(0, T; H^{-1}(\Omega)),$$

$$\chi(\text{tr}(\mathbf{C}))\mathbf{C} \in L^{\frac{4}{3}}(\Omega_T), \quad \Phi(\text{tr}(\mathbf{C})) \in L^2(\Omega_T), \quad \text{for any } 1 \leq q < 2$$

- *the energy inequality holds a.e. $t \in (0, T)$*

$$\begin{aligned} & \left(\int_{\Omega} \frac{1}{2} |\mathbf{u}(t)|^2 + \frac{1}{4} |\text{tr}(\mathbf{C}(t))|^2 \, dx \right) + \int_0^t \int_{\Omega} \eta |\nabla \mathbf{u}|^2 + \frac{\varepsilon}{2} |\nabla \text{tr}(\mathbf{C})|^2 \, dx \, d\tau + \\ & \int_0^t \int_{\Omega} \frac{1}{2} |\text{tr}(\mathbf{C})|^4 + \frac{a}{2} |\text{tr}(\mathbf{C})|^3 \, dx \, d\tau \\ & \leq \int_0^t \int_{\Omega} \frac{1}{2} |\text{tr}(\mathbf{C})|^2 + \frac{a}{2} \text{tr}(\mathbf{C}) \, dx \, d\tau + \left(\int_{\Omega} \frac{1}{2} |\mathbf{u}(0)|^2 + \frac{1}{4} |\text{tr}(\mathbf{C}(0))|^2 \right) \end{aligned}$$

- If $a = 0$ the conformation tensor \mathbf{C} is symmetric positive semi-definite
- If $a > 0$ and $\text{tr}(\log \mathbf{C}_0) \in L^1(\Omega)$ then \mathbf{C} is symmetric positive definite and

$$\begin{aligned}\text{tr}(\log \mathbf{C}) &\in L^\infty(0, T; L^1(\Omega)) \cap L^2(0, T; H^1(\Omega)), \\ \text{tr}(\mathbf{C}^{-1}), \text{tr}(\mathbf{C}^{-1})\text{tr}(\mathbf{C}) &\in L^1(0, T; L^1(\Omega)).\end{aligned}$$

$$\begin{aligned}& \left(\int_{\Omega} \frac{1}{2} |\mathbf{u}(t)|^2 + \frac{1}{4} |\text{tr}(\mathbf{C}(t))|^2 - \frac{1}{2} \text{tr}(\log \mathbf{C}(t)) \, dx \right) \\ &+ \int_0^t \int_{\Omega} \eta |\nabla \mathbf{u}|^2 + \frac{\varepsilon}{2} |\nabla \text{tr}(\mathbf{C})|^2 + \frac{\varepsilon}{6} |\nabla \text{tr}(\log \mathbf{C})|^2 + \frac{1}{2} \chi(\text{tr}(\mathbf{C})) \text{tr}(\mathbf{T} + \mathbf{T}^{-1} - 2\mathbf{I}) \, dx \, d\tau \\ &\leq \left(\int_{\Omega} \frac{1}{2} |\mathbf{u}(0)|^2 + \frac{1}{4} |\text{tr}(\mathbf{C}(0))|^2 - \frac{1}{2} \text{tr}(\log \mathbf{C}(0)) \, dx \right).\end{aligned}$$

Hybrid kinetic-macroscopic model

- Fokker-Planck equation for the viscoelastic part

$$\partial_t \phi + \mathbf{u} \cdot \nabla_{\mathbf{x}} \phi = \operatorname{div}_{\mathbf{x}} \left((1 + \varepsilon_0) m(\phi) \nabla_{\mathbf{x}} \mu - m^{1/2}(\phi) \nabla_{\mathbf{x}} (A(\phi) q) \right),$$

$$\mu = -\gamma \Delta_{\mathbf{x}} \phi + f'(\phi),$$

$$\partial_t q + \mathbf{u} \cdot \nabla_{\mathbf{x}} q = -\frac{1}{\tau(\phi)} q + \varepsilon_1 \Delta_{\mathbf{x}} q + A(\phi) \operatorname{div}_{\mathbf{x}} \left(\nabla_{\mathbf{x}} (A(\phi) q) - m^{1/2}(\phi) \nabla_{\mathbf{x}} \mu \right),$$

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla_{\mathbf{x}}) \mathbf{u} = \operatorname{div}_{\mathbf{x}} (\eta(\phi) D_{\mathbf{x}} \mathbf{u} - p \mathbf{I} + \mathbf{T}(\psi)) - \phi \nabla_{\mathbf{x}} \mu,$$

$$\operatorname{div}_{\mathbf{x}} (\mathbf{u}) = 0,$$

$$\mathbf{T}(\psi) = \gamma_3 (\langle |\mathbf{R}|^2 \rangle) \langle \mathbf{R} \otimes \mathbf{R} \rangle,$$

$$\partial_t \psi + \mathbf{u} \cdot \nabla_{\mathbf{x}} \psi + \operatorname{div}_{\mathbf{R}} (\nabla_{\mathbf{x}} \mathbf{u} \mathbf{R} \psi)$$

$$= \gamma_2 (\phi, \langle |\mathbf{R}|^2 \rangle) \Delta_{\mathbf{R}} \psi + \operatorname{div}_{\mathbf{R}} (\gamma_1 (\phi, \langle |\mathbf{R}|^2 \rangle) \mathbf{R} \psi) + \varepsilon_2 \Delta_{\mathbf{x}} \psi$$

$\gamma_1, \gamma_2, \gamma_3$ are connected to the functions χ, Φ in the Peterlin model

$\langle f \rangle \equiv \int_{R^3} f(\mathbf{R}) \psi(\mathbf{x}, t, \mathbf{R}) d\mathbf{R} \dots \psi$ is the probability density distribution

$\mathbf{C}(\psi) \equiv \langle \mathbf{R} \otimes \mathbf{R} \rangle$

Existence of weak solutions for the kinetic system

► Existence of weak solutions for the kinetic system

Let $d = 2$ and assume that $\gamma_1(s) = s^2, \gamma_2(s) = s, \gamma_3(s) = s$.

- ① Then there exists at least one global weak solution of the hybrid kinetic-macroscopic viscoelastic phase separation model.
- ② **Rigorous macroscopic closure:** the macroscopic viscoelastic phase separation model (Cahn-Hilliard-Navier-Stokes-Peterlin) is the closure of the hybrid kinetic-macrosopic model
- ③ $\mathbf{C} = \langle \mathbf{R} \otimes \mathbf{R} \rangle$