Lipid rafts on cell membranes: modeling and analysis

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FWF ESPRIT Grant n. ESP 552

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Alexander von Humboldt Research Fellow

Prague, February 5-7, 2025 - EMS TAG **MIXTURES**:

Mixtures: Modeling, analysis and computing

1. Introduction
   - Biological applications
2. Mathematical models for prescribed surface evolution
   - Evolving surface setting
   - Binary fluids on evolving surfaces
3. Perspectives

Cell membranes and lipid rafts

- **Eukaryotic cell membranes** consist of a heterogeneous but regulated environment serving as a **dynamic platform** for cell functions
- **Membrane heterogeneity** includes **discrete** membrane **domains**:

Lipid rafts

⇓

Cholesterol associations with membrane lipids like **sphingolipids**

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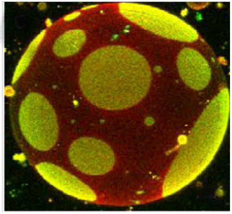
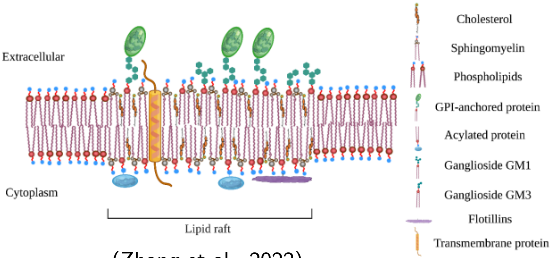


(Morales-Penningston et al., 2010)

Cell membranes and lipid rafts

- **Lipid rafts** believed to play an **essential role** in the **regulation** of **protein activity**
- Known to be **central** to the **replication** of some **viruses** like **HIV**
- Liquid **ordered** phase VS liquid **disordered** phase:

Liquid-Liquid Phase Separation on the cell **membrane**



(Zhang et al., 2022)

The domain of the model equations

- **Changing cell shape** is crucial for the proper function of cellular processes, including **cell migration** (e.g., lymphocytes and stem cells)
- **Lipid rafts** formation **changes the shape** of the cell membranes: the shape **depends** on **local inhomogeneities** within the membrane
- **Essential** to consider

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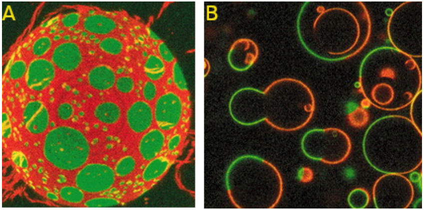

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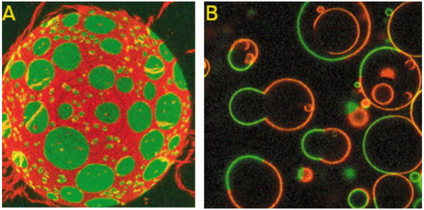

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The evolving surface setting

- $t \in [0, T]$, $T > 0$, evolving time
- Γ_0: initial **closed** surface of a (regular) liposome, diameter 10 μm
- $\Phi : [0, T] \times \Gamma_0 \to \mathbb{R}^3$, a sufficiently smooth **flow map** characterizing the evolution of Γ_0
- $\Gamma(t) := \Phi(t, \cdot)$ so that $\Phi_t^0 := \Phi(t, \cdot) : \Gamma_0 \to \Gamma(t)$
- $\mathbf{V_n}$: normal velocity field s.t., for any $t \in [0, T]$, for any $x \in \Gamma_0$,

$$\frac{d}{dt}\Phi_t^0(x) = \mathbf{V_n}(t, \Phi_t^0(x))$$
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A phase-field model for binary fluids on evolving surfaces

- $\varphi \in [-1,1]$: **relative concentration difference** between the ordered and disordered phases (diffuse interface)
- We consider

$$\mu := -\Delta_{\Gamma(t)}\varphi + \Psi'(\varphi), \qquad \textbf{chemical potential}$$

✓ Ψ: Flory Huggins **free energy** density (potential), $0 < \theta < \theta_0$

$$\Psi(\varphi) = \underbrace{\frac{\theta}{2}((1+\varphi)\ln(1+\varphi) + (1-\varphi)\ln(1-\varphi))}_{F(\varphi):\ \text{convex and logarithmic}} - \frac{\theta_0}{2}\varphi^2$$

- $\partial^\circ\varphi$ **normal** material **time derivative**

A phase-field model for binary fluids on evolving surfaces

- Introduce a model for $\mathbf{u}$ as **tangential fluid velocity**
- **Incompressible** two-phase **fluid**: for any $t \in [0, T]$

$$\mathrm{div}_{\Gamma(t)}(\underbrace{\mathbf{V_n} + \mathbf{u}}_{\text{Total fluid velocity}}) \equiv 0 \quad \text{on } \Gamma(t)$$

- This also entails **inextensible material surface** assumption:

$$\int_{\Gamma(t)} \mathrm{div}_{\Gamma(t)} \mathbf{V_n} = \int_{\Gamma(t)} H(\mathbf{V_n} \cdot \mathbf{n}) = 0$$

- **Unmatched** fluid viscosities $\nu = \nu(\varphi)$ and densities $\rho = \rho(\varphi)$
- **Thermodynamically consistent model** following a similar **derivation** as in Abels-Garcke-Grün (2012)

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Binary fluids on evolving surfaces: the model

- $\mathbf{P}(x,t)$: normal **projector** on the **tangential space** at $x \in \Gamma(t)$
- $\nabla_{\Gamma(t)}\mathbf{u}$: covariant derivative of $\mathbf{u}$
- Introduce:

$$v_{\mathbf{n}} := \mathbf{V}_{\mathbf{n}} \cdot \mathbf{n}, \quad \mathbf{H} := \nabla_{\Gamma(t)}\mathbf{n},$$

$$H := \operatorname{tr} \mathbf{H} \quad \Longrightarrow \quad \text{double mean curvature}$$

$$\mathcal{E}_S(\mathbf{u}) := \frac{1}{2}(\nabla_{\Gamma(t)}\mathbf{u} + \nabla_{\Gamma(t)}^T\mathbf{u})$$

$$\nu(\varphi) := \nu_1\frac{1+\varphi}{2} + \nu_2\frac{1-\varphi}{2}$$

$$\rho(\varphi) = \rho_1\frac{1+\varphi}{2} + \rho_2\frac{1-\varphi}{2}$$

$$\mathbf{J}_\rho = -\frac{\rho_1-\rho_2}{2}\nabla_{\Gamma(t)}^T\mu \quad \Longrightarrow \quad \text{extra } \textbf{flux} \text{ term}$$

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Binary fluids on evolving surfaces: the model

- Assuming that the velocity $\mathbf{V}_\mathbf{n}$ is *a priori* **prescribed**, consider **only** the projected equation for $\mathbf{u}$
- Find $(\mathbf{u}, p, \varphi)$ such that, for any $(x,t) \in \bigcup_{t\in[0,T]} \Gamma(t) \times \{t\}$,

$$
\begin{cases}
\rho \mathbf{P} \partial^\circ \mathbf{u} + ((\rho \mathbf{u} + \mathbf{J}_\rho) \cdot \nabla_{\Gamma(t)}) \mathbf{u} + \rho v_\mathbf{n} \mathbf{H} \mathbf{u} + v_\mathbf{n} \mathbf{H} \mathbf{J}_\rho \\
-2\mathbf{P}\mathrm{div}_{\Gamma(t)}(\nu(\varphi)\mathcal{E}_S(\mathbf{u})) + \nabla_{\Gamma(t)} p \\
= -\mathbf{P}\mathrm{div}_{\Gamma(t)}(\nabla_{\Gamma(t)}\varphi \otimes \nabla_{\Gamma(t)}\varphi) + 2\mathbf{P}\mathrm{div}_{\Gamma(t)}(\nu(\varphi) v_\mathbf{n} \mathbf{H}) + \frac{\rho}{2}\nabla_{\Gamma(t)}(v_\mathbf{n})^2, \\
\mathrm{div}_{\Gamma(t)}\mathbf{u} = -\mathrm{div}_{\Gamma(t)}\mathbf{V}_\mathbf{n} = -H v_\mathbf{n}, \\
\\
\partial^\circ \varphi + \mathbf{u} \cdot \nabla_{\Gamma(t)}\varphi = \Delta_{\Gamma(t)}\mu, \\
\mu = -\Delta_{\Gamma(t)}\varphi + \Psi'(\varphi), \\
\mathbf{u}(0) = \mathbf{u}_0, \quad \varphi(0) = \varphi_0
\end{cases}
$$

Main result (Abels-Garcke-P., 2024)

- Assume $\mathbf{V_n}$ and $(\mathbf{u}_0, \varphi_0)$ **sufficiently regular**
- **Well-posedness** of **global strong** solutions on $[0, T]$ such that

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\begin{aligned}
&\mathbf{u} \in L^\infty_{\mathbf{L}^2} \cap L^2_{\mathbf{H}^2} \cap H^1_{\mathbf{L}^2}, \quad p \in L^2_{H^1}, \\
&\varphi \in L^\infty_{H^3} \cap L^2_{H^4} \cap H^1_{H^1}, \\
&|\varphi| < 1 \quad \text{a.e. in } \Gamma(t) \quad \text{for a.a. } t \in [0, T], \\
&\mu \in L^\infty_{H^1} \cap L^2_{H^3} \cap H^1_{H^{-1}},
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$$

- Instantaneous **strict separation property**:

$$
\exists \delta > 0 : \quad \sup_{t \in [0,T]} \|\varphi\|_{L^\infty(\Gamma(t))} \leq 1 - \delta
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- **Questions**: **minimal assumptions** on Ψ to get **separation**? Do we need φ_0 **strictly separated**?

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Classical approach: Moser-Trudinger (MT) inequality

We assume as in the **logarithmic potential**:

$$F''(s) \leq Ce^{C|F'(s)|}, \qquad \forall s \in (-1,1)$$

Variant of Moser-Trudinger inequality on Γ_0 (Fontana, 1993)

It holds:

$$\int_{\Gamma_0} e^{|f|} \leq C(\Gamma_0)e^{C\|f\|^2_{H^1(\Gamma_0)}}, \qquad \forall f \in H^1(\Gamma_0),$$

- Use this inequality on the pullback of $F''(\varphi)$ on Γ_0 to get $F''(\varphi) \in L^\infty_{L^p}$, $\quad \forall p \in [2,\infty)$

☺ **Strict separation property** holds (Caetano-Elliott-Grasselli-P.,2023)

An alternative to MT inequality: De Giorgi iterations

- **New assumption** (Gal & P., 2024): as $\delta \to 0^+$

$$\exists \gamma > \frac{1}{2}: \quad \frac{1}{F'(1-2\delta)} = O\left(\frac{1}{|\ln(\delta)|^\gamma}\right), \quad \frac{1}{|F'(-1+2\delta)|} = O\left(\frac{1}{|\ln(\delta)|^\gamma}\right)$$

✓ Use of **De Giorgi iteration** scheme for the **elliptic equation**:

$$\mu(t) = -\Delta_{\Gamma(t)}\varphi(t) + \Psi'(\varphi(t))$$

✓ More **geometric** approach to obtain

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Strict separation of the initial datum φ_0

- **Regularity assumptions** to get **strong solutions**:

$$\varphi_0 \in H^2(\Gamma_0), \quad |\varphi_0| \leq 1, \quad -1 < \frac{\int_{\Gamma_0} \varphi_0}{|\Gamma_0|} < 1,$$

$$\mu_0 := -\Delta_{\Gamma_0}\varphi_0 + \Psi'(\varphi_0) \in H^1(\Gamma_0)$$

- **Repeat** the **De Giorgi**'s iteration **scheme** on μ_0
- We can prove that φ_0 is **automatically strictly separated**, i.e.,

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Further developments

- ***A priori*** **given** normal velocity $\mathbf{V_n}$:
  - Extension to **multi-component** phase-field models
  - Applications to **optimal control** problems
- **Not** ***a priori*** **given** velocity:
  - **Geometric evolution** is part of the **problem**
  - **Navier-Stokes systems** (Jankuhn et al., 2018) for **inextensible** viscous materials:

$$\begin{cases} \partial^\bullet \mathbf{v} = -\nabla_{\Gamma(t)}\pi + 2\nu \,\mathrm{div}_{\Gamma(t)}\mathcal{E}_S(\mathbf{v}) + \pi H\mathbf{n}, \\ \mathrm{div}_{\Gamma(t)}\mathbf{v} = 0, \quad \mathbf{v_n} = \mathbf{v}\cdot\mathbf{n} \end{cases}$$

with $\mathbf{v}$ velocity field of the **flow** on $\Gamma(t)$ and $\partial^\bullet$ material **time derivative** with respect to $\mathbf{v}$

$\Longrightarrow$ **Not enough regularity** to **close** the estimates for $v_{\mathbf{n}}$ due to the **coupling with** π

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    $\Longrightarrow$ **regularizing** elastic term $-\Delta_{\Gamma(t)} H$ in the equation for $v_{\mathbf{n}}$

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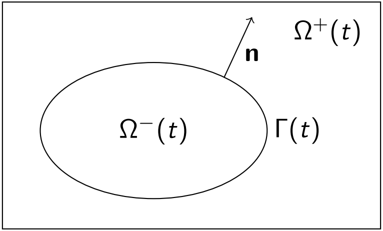
Short-time Existence of **strong solutions**
(Abels-Liu-P., 2025)

Further developments



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  - **Strong solutions** can in general only be **local** in time
  - From local-in-time to **global-in-time**:
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Navier-Stokes-Mullins-Sekerka flow (Abels-P., 2025)

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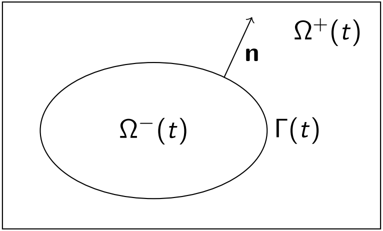

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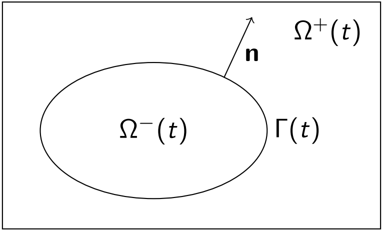

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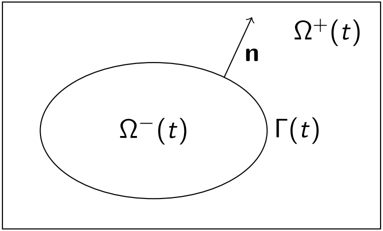

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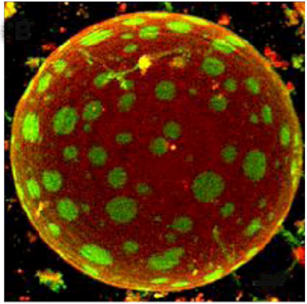
  - **Weak-strong uniqueness** results

Thanks for your attention!



(Morales-Penningston et al., 2010)

Essential bibliography

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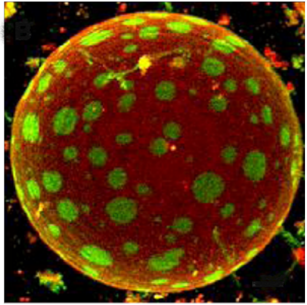
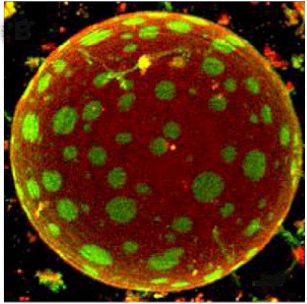
Thanks for your attention!



(Morales-Penningston et al., 2010)

Thanks for your attention!



(Morales-Penningston et al., 2010)

Navier-Stokes on elastic membranes

$$
\begin{cases}
\rho \mathbf{P} \partial^{\bullet} \mathbf{v} \\
\quad = -\nabla_{\Gamma}\pi + \mu(\Delta_{\Gamma}\mathbf{v} + K\mathbf{v} + \nabla_{\Gamma}(v_{\mathbf{n}}H) - 2(H\mathbf{P} - \mathbf{H})\nabla_{\Gamma}v_{\mathbf{n}}) - \rho v_{\mathbf{n}} \cdot \partial^{\bullet}\mathbf{n} \\
\\
\rho \partial^{\bullet} v_{\mathbf{n}} = -2\mu(\mathrm{tr}(\mathbf{H}\nabla_{\Gamma}\mathbf{v}) + v_{\mathbf{n}}\mathrm{tr}(\mathbf{H}^2)) + \pi H + \rho \partial^{\bullet}\mathbf{n} \cdot \mathbf{v} \\
\qquad + C_H(\Delta_{\Gamma}H + H(H^2/2 - 2K) + H_0(2K - HH_0/2)) \\
\\
\mathrm{div}_{\Gamma}\mathbf{v} = -v_{\mathbf{n}}H \\
\partial^{\bullet}\rho = 0
\end{cases}
$$

where $\mathbf{H} = \nabla_{\Gamma}\mathbf{n}$, K is the **Gauß curvature**, H_0, K_0 are **positive constants**, and the **velocity** of the material surface is $\mathbf{v} + v_{\mathbf{n}}\mathbf{n}$

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Cahn-Hilliard and Navier-Stokes on evolving surfaces

A priori **prescribed evolution** of the surface: **weak** solutions

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