Non-equilibrium thermodynamics and hydrodynamics of lipid membranes

DOE CSGF Program Review

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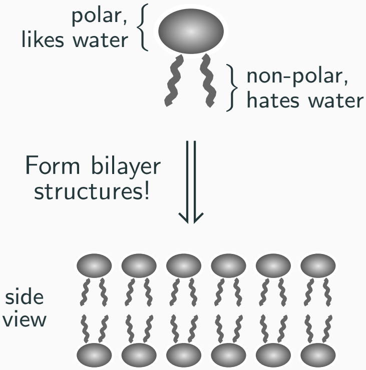
13–15 July 2020

University of California, Berkeley

Introduction to lipid membranes: structure and behavior



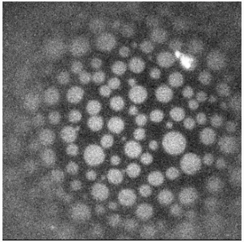
Lipid membranes in the cell:

Make up the exterior cell membrane and boundary of the nucleus, Golgi complex, endoplasmic reticulum. . .

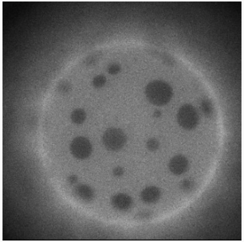
Constitutive behavior

Lipid membranes are **fluid in-plane** and **elastic out-of-plane**

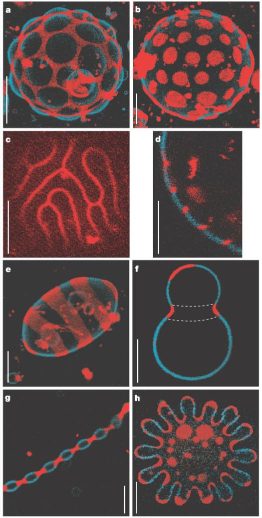
Experimental observations: Phase separation, chemical reactions



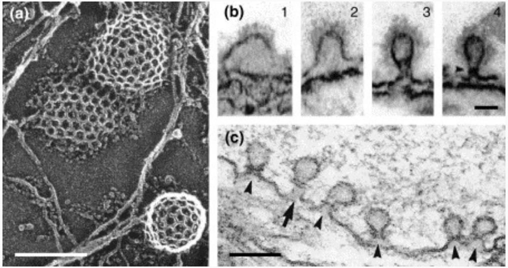
Honerkamp-Smith et al. 2012



Stanich et al. 2013



Baumgart, Hess, Webb 2003



McMahon et al. 2002

We observe coupling between:

- in-plane lipid flow, out-of-plane bending
- in-plane diffusion of different species
- protein binding chemical reactions from surrounding fluid

Modeling lipid membranes: How do we . . .

. . . model phenomena over 200 nm–10μm and several seconds?

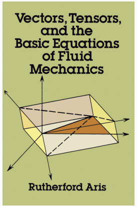
Use the balance law formalism of continuum mechanics

. . . describe the different shapes and morphologies lipid membranes form?

Write the equations of motion in a differential geometric setting

. . . understand the complex coupling between bending and various irreversible processes?

Develop an irreversible thermodynamic framework to determine the stresses and fluxes in the system



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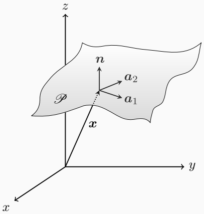

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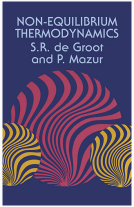
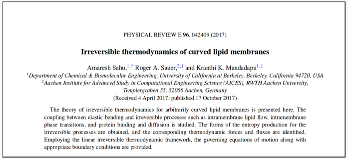


$\Rightarrow$



PHYSICAL REVIEW E **96**, 042409 (2017)

Irreversible thermodynamics of curved lipid membranes

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(Received 4 April 2017; published 17 October 2017)

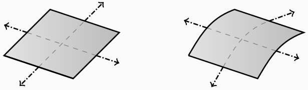
The theory of irreversible thermodynamics for arbitrarily curved lipid membranes is presented here. The coupling between elastic bending and irreversible processes such as intramembrane lipid flow, intramembrane phase transitions, and protein binding and diffusion is studied. The forms of the entropy production for the irreversible processes are obtained, and the corresponding thermodynamic forces and fluxes are identified. Employing the linear irreversible thermodynamic framework, the governing equations of motion along with appropriate boundary conditions are provided.

arXiv:1701.06495, *Phys. Rev. E* **96** (2017)

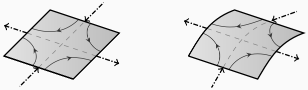
Viscous forces in the normal direction ⇒ new dimensionless number!

Membrane shape equation:

$$0 = p + \underbrace{2\lambda H}_{\text{surface tension}} - \underbrace{2k_b H(H^2 - K) - k_b \Delta H}_{\text{bending}} + \underbrace{\pi^{\alpha\beta} b_{\alpha\beta}}_{\text{viscous–curvature coupling}}$$



(a) tension forces: $2\lambda H$



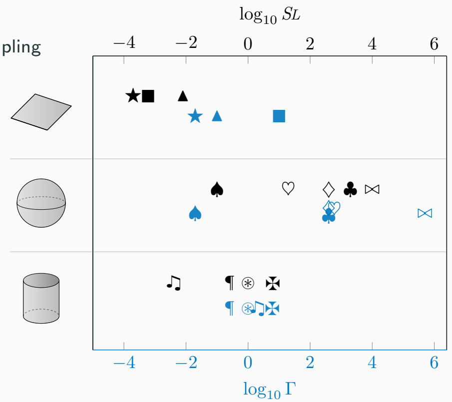
(b) viscous forces: $\pi^{\alpha\beta} b_{\alpha\beta}$

Föppl–von Kármán #

$$\Gamma = \frac{O(2\lambda H)}{O(k_b \Delta_s H)} = \frac{\lambda L^2}{k_b}$$

Scriven–Love #

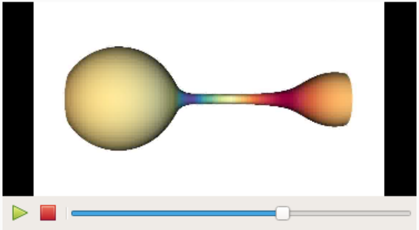
$$SL = \frac{O(\pi^{\alpha\beta} b_{\alpha\beta})}{O(k_b \Delta_s H)} = \frac{\zeta V L}{k_b}$$



arXiv:1910.10693 *Phys. Rev. E* **101** (2020)

Lipid membrane tubes are unstable at large Föppl–von Kármán number!

Fluid film: $k_b = 0,\ \Gamma \to \infty$



arXiv:1812.05086, *J. Comp. Phys.* **407** (2020)

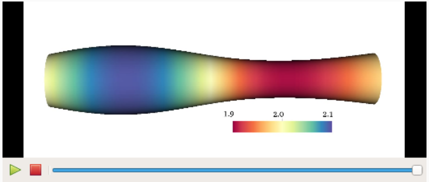
Physical mechanism:

1. initial shape change causes a change in the surface tension (Young–Laplace equation)
2. resultant surface tension gradients drive in-plane flows, from low to high tension

Important result:

1. when $k_b \neq 0$, bending and tension forces are *competing* in the normal direction
2. we investigate both the *mechanism* and the *dynamics* of the pearling instability!

Lipid membrane $k_b \neq 0,\ \Gamma = 2$:



Acknowledgements and Summary

$$0 = p + \underbrace{2\,\lambda\,H}_{\text{surface tension}} - \underbrace{2k_{\mathrm{b}} H\left(H^2 - K\right) - k_{\mathrm{b}}\Delta H}_{\text{bending}} + \underbrace{2\zeta b^{\alpha\beta} v_{\alpha;\beta} - 4\zeta v\left(2H^2 - K\right)}_{\text{viscous–curvature coupling}}$$

Scriven–Love number: $S\!L = \dfrac{\zeta V L}{k_{\mathrm{b}}}$

References: amaresh-sahu.github.io

- Irreversible thermodynamics: *arXiv:1701.06495*, *PRE* **96** (2017)
- Non-dimensionalization: *arXiv:1910.10693*, *PRE* **101** (2020)
- Simulating fluid films: *arXiv:1812.05086*, *JCP* **704** (2020)

In prep: Simulating lipid membranes

Thank you for your support!

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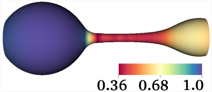

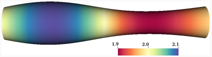

People: