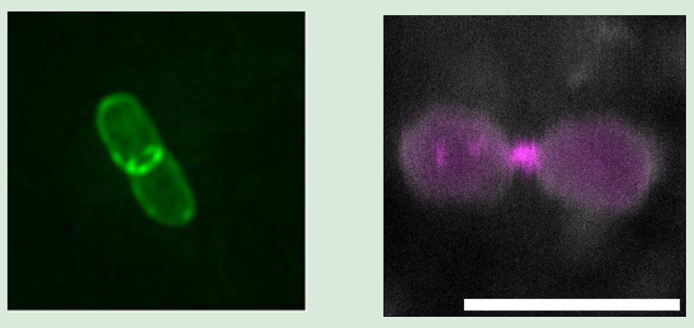
Exploring the physics of Synthetic Cell Division

Modeling and Simulating Lipid Bilayer Membrane Dynamics

Pietro Sillano[1], Siewert-Jan Marrink[2], Timon Idema[1]
[1]Kavli Institute of Nanoscience, Dpt. of Bionanoscience, TU Delft
[2]Faculty of Science and Engineering, Rijksuniversiteit Groningen
p.sillano@tudelft.nl

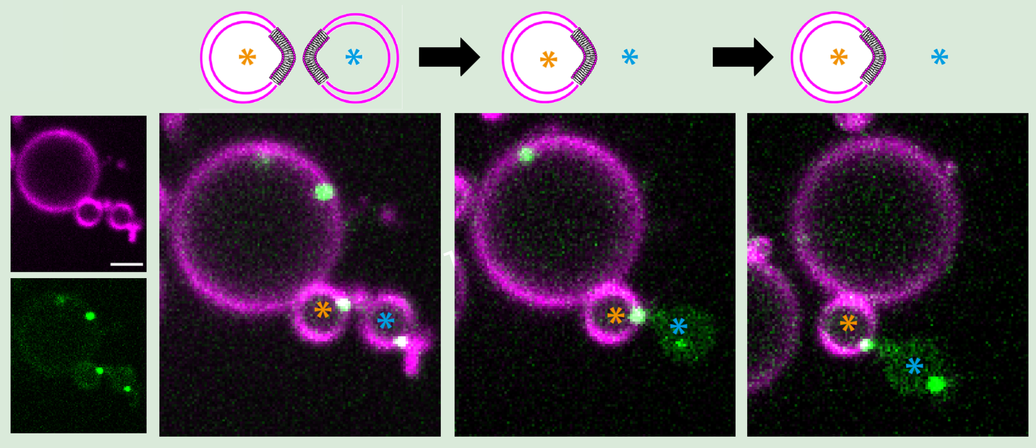
FtsZ approach



From Ramirez F. [8]

Liposome constriction only

Dynamin approach



From De Franceschi [1]

Liposomes division but still proof of concept

Membrane reshaping → Successful division ← Active constriction process

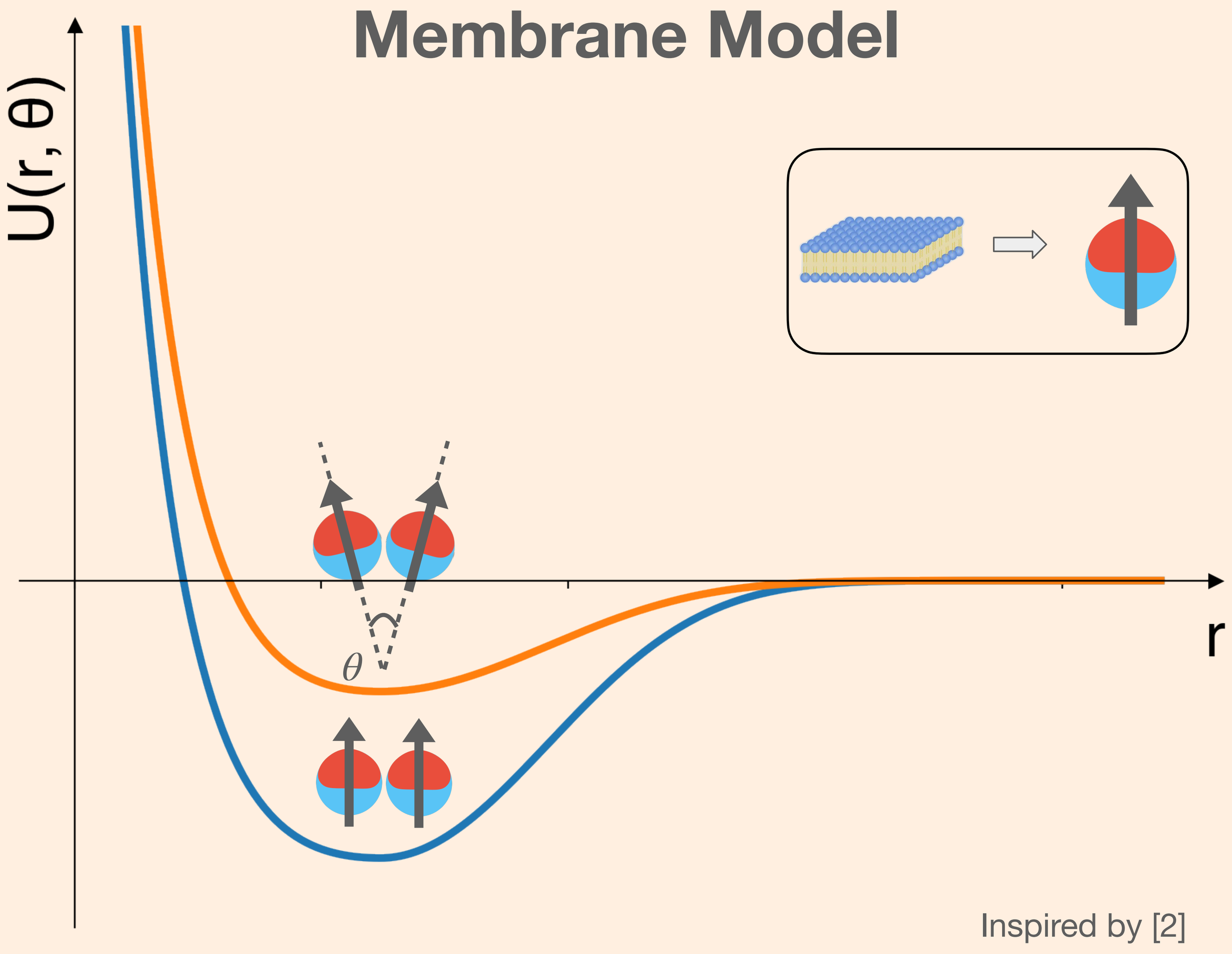
Under which **conditions** could liposomes divide?

Which **active** mechanisms are involved in this process?

⟺

Computer experiment can help to design and guide lab experiments

Membrane Model



Inspired by [2]

Interaction weighted by relative beads **orientation** ⟹ **Effective** hydrophobic interaction

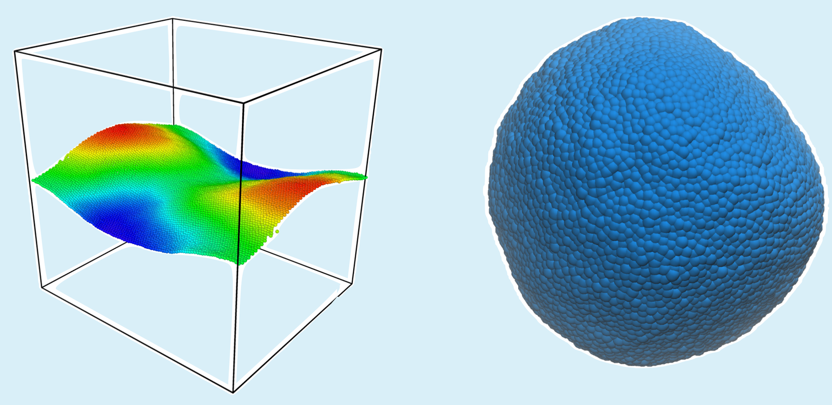
Implicit solvent ⟹ Langevin dynamics

$$m\dot{\mathbf{v}} = \mathbf{F} - \gamma \mathbf{v} + \boldsymbol{\eta}$$
$$I\dot{\omega} = \mathbf{T} - \gamma_r \omega + \boldsymbol{\eta}_r$$

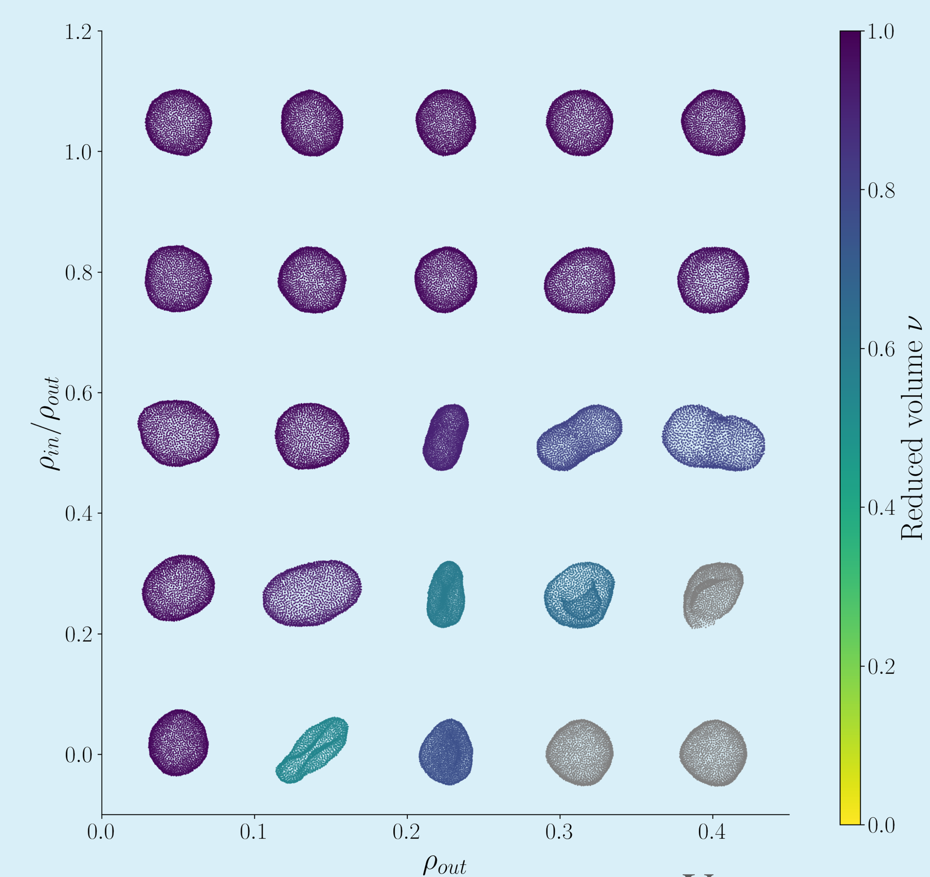
Relevant scales

Time	0.1 - 100 μs
Size	100 nm - 10 μm
Bending rigidity	10 - 100 K_BT

Membrane fluctuations



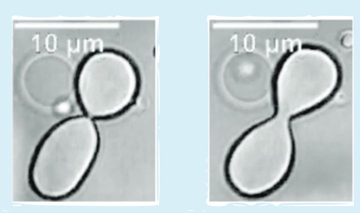
Shape diagram



$$R_{ve} = \sqrt{\frac{A}{4\pi}} \qquad \nu = \frac{V}{\frac{4}{3}\pi R_{ve}^3}$$

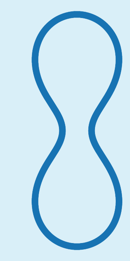
Coupling spontaneous curvature

Min protein system



From Christ [3]

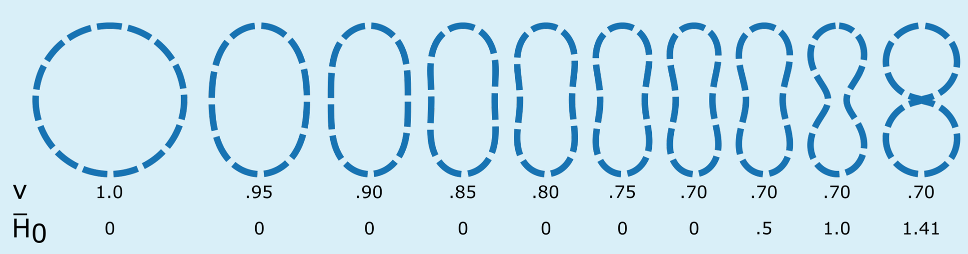
Theory



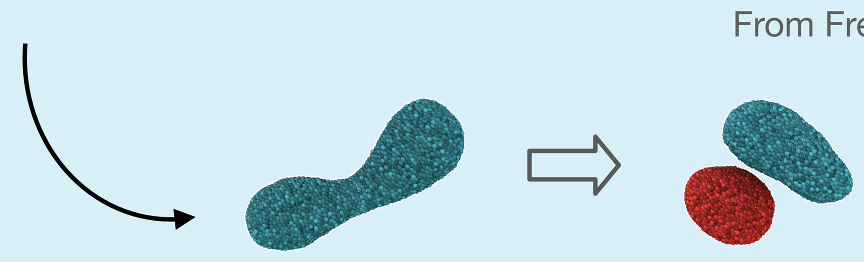
From Frey [4]

Simulation

Sequential change of volume and spontaneous curvature:



From Frey [4]

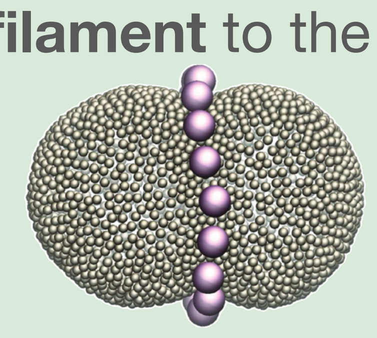


Unstable state

What's next?

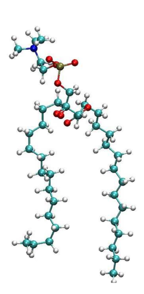
Include **tilt** degree of freedom of lipids in the membrane model [5]

Self assembly and binding of an **active filament** to the membrane

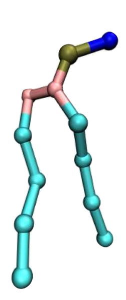


Adapted from [6]

Spatial and temporal scales

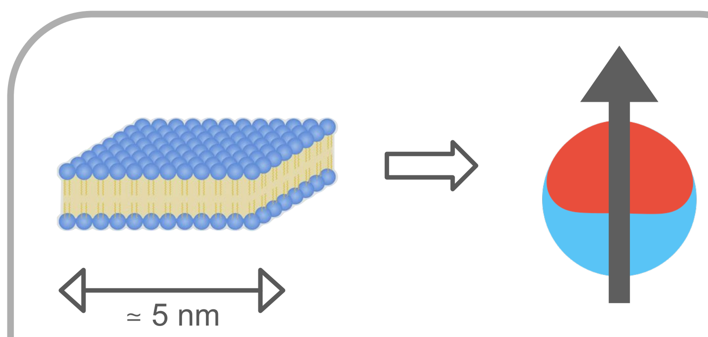


Atomistic

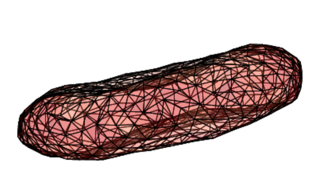


Coarse grain

Unaccessible time and spatial scales

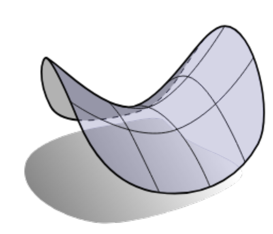


Super CG or Mesoscopic



MC Dynamic triangulated surface: Flippy [7]

Topology change



Continuum models

Simple toy models

Microscopic ⟶ Macroscopic

[1] N. De Franceschi, Nat. Nanotechnol. (2023).
[2] H. Yuan, Phys. Rev. E (2010).
[3] S. Christ, Soft Matter (2021).
[4] F. Frey, Phys. Rev. E (2022).
[5] H. Noguchi, The Journal of Chemical Physics (2011).
[6] A. Vahid, Soft Matter (2017).
[7] G. Dadunashvili, arXiv:2303.12305.
[8] F. Ramirez, photo, Koenderink Lab

TU Delft / university of groningen / BaSyC