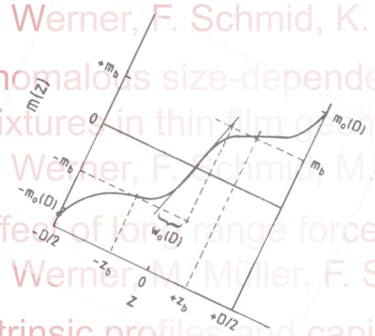
Simulation of condensed matter

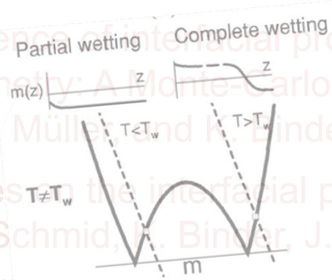
Session in memory of Prof. Kurt Binder

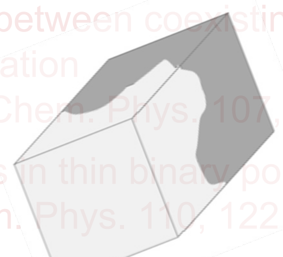
My own (paper) history with Kurt Binder

List of joint research papers (except proceedings)

- Modelling order-disorder and magnetic transitions in iron-aluminium alloys
  F. Schmid, K. Binder, J. Phys.: Cond. Matter 4, 3569 (1992).
- Monte Carlo investigation of interface roughening in a bcc-based binary alloy
  F. Schmid, K. Binder, Phys. Rev. B 46, 13565 (1992).
- Diblock copolymers at a homopolymer-homopolymer interface: A Monte Carlo simulation
  A. Werner, F. Schmid, K. Binder, M. Müller, Macromolecules 29, 8241 (1996).
- Anomalous size-dependence of interfacial profiles between coexisting phases of polymer mixtures in thin film geometry: A Monte-Carlo simulation
  A. Werner, F. Schmid, M. Müller, and K. Binder, J. Chem. Phys. 107, 8175 (1997).
- Effect of long-range forces on the interfacial profiles in thin binary polymer films
  A. Werner, M. Müller, F. Schmid, K. Binder, J. Chem. Phys. 110, 1221 (1999).
- Intrinsic profiles and capillary waves at homopolymer interfaces: A Monte Carlo study
  A. Werner, F. Schmid, M. Müller, K. Binder, Phys. Rev. E 59, 728 (1999).
- Interfacial profiles between coexisting phases in thin films: Cahn-Hilliard treatment versus capillary waves
  K. Binder, M. Müller, F. Schmid, A. Werner, J. Stat. Phys. 95, 1045 (1999).
- Surface induced disorder in body-centered cubic alloys
  F.F. Haas, F. Schmid, K. Binder, Phys. Rev. B 61, 15077 (2000).
- Critical behavior of active Brownian particles
  J.T. Siebert, F. Dittrich, F. Schmid, K. Binder, T. Speck, P. Virnau, Phys. Rev. E 98, 030601(R) (2018).







Mostly on Interfaces

Strong Focus on Statistical Physics

Simulation of condensed matter

Session in memory of Prof. Kurt Binder

Simulation of condensed matter

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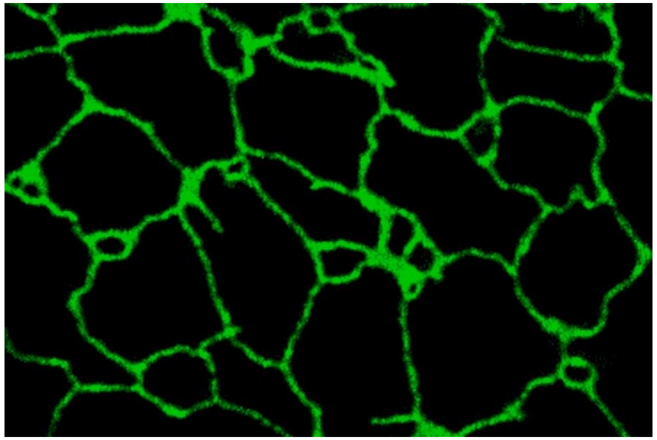
Simulations of branched tubular membrane structures

Friederike Schmid, Universität Mainz

Maike Jung, Gerhard Jung

Tubular membrane structures in cells

Endoplasmatic reticulum



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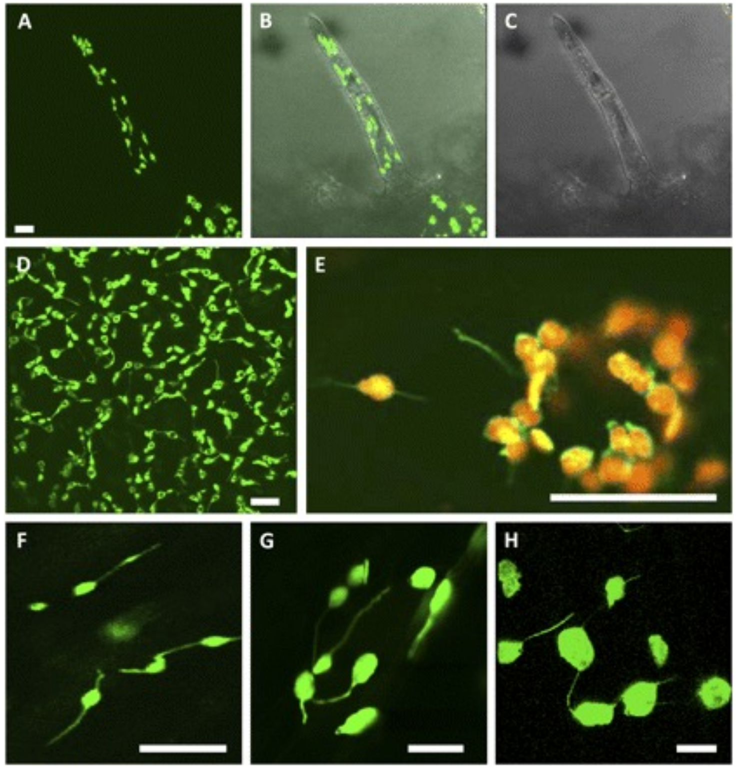
Plastides and stromulae

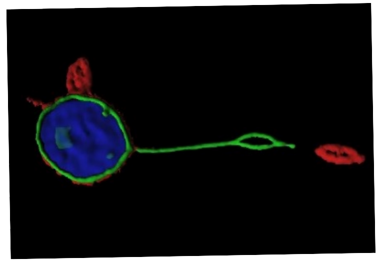


Hanson, Sattarzadeh
Plant Physiol. 2011;155:1486-1492

Tubular structures – Stabilization?

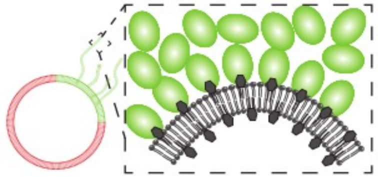
- Curvature active membrane proteins

  (z.B. Machettira … Schleiff Frontiers Plant Science 2012)



- "Protein crowding"

  (Stachowiak et al, Nature Cell Biol. 2012)



- Interactions with membranes of other organelles

  (Schattat et al, Plant Physiology 2011)

- Active mechanism, mechanic force due to cytoplasm

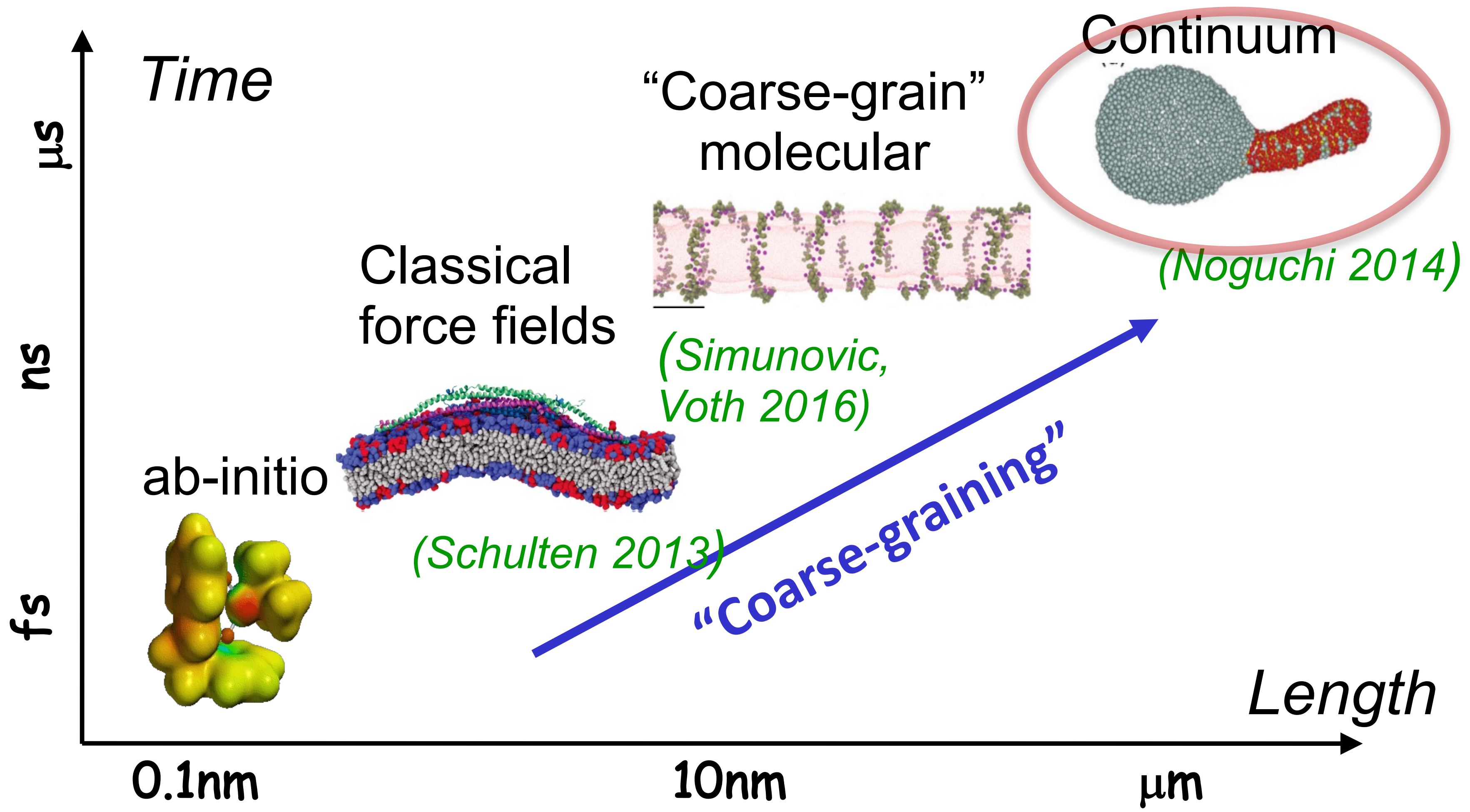
  (Kwok, Hanson, Plant Journal 2003)

Question:

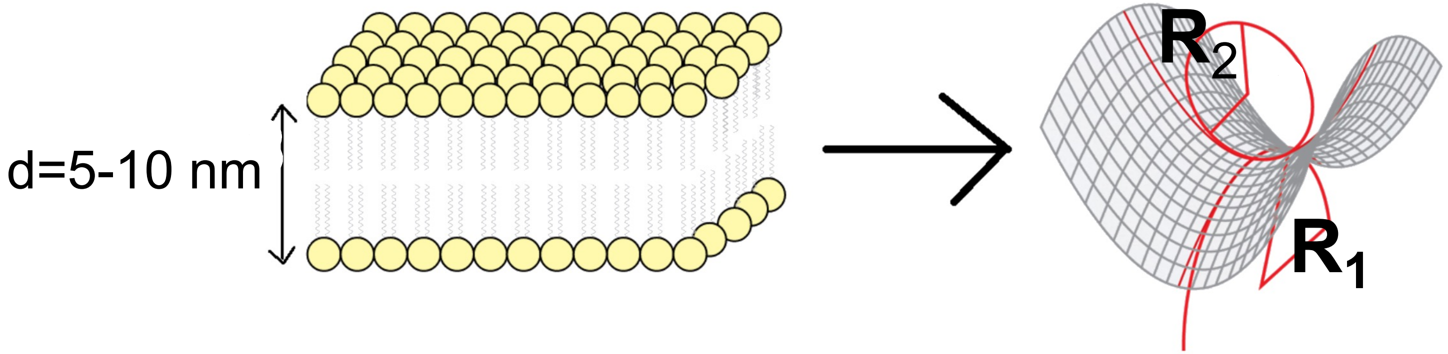
Is there anything we can learn from simple models?

Characteristic length scales in membranes

Example: Membrane tubulation due to BAR-proteins



Minimal model of membrane shapes



- **Elastic "Helfrich" Energy** (simplest variant)

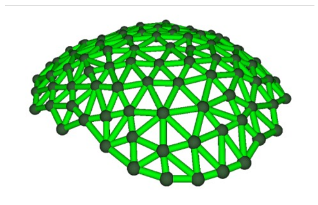
$$F = \int \mathrm{d}\mathbf{A} \left\{ \frac{\kappa}{2}(K - K_0)^2 + \kappa_G K_G \right\}$$

$K = 1/R_1 + 1/R_2$: Total curvature

$K_G = 1/(R_1 R_2)$: Gaussian curvature

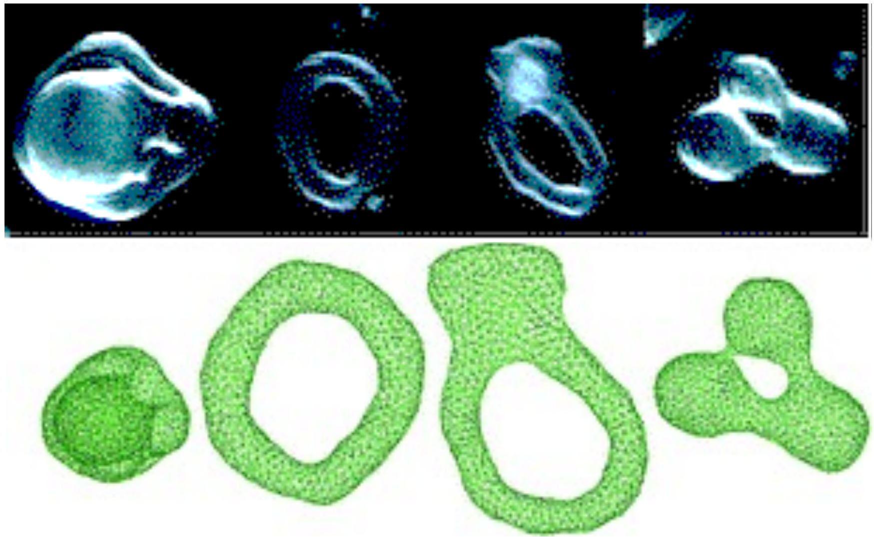
- Elastic parameters κ, κ_G, c_0 depend on membrane
- **Simulation**: Triangulated membrane model

(Noguchi, Gompper, Phys. Rev. E 2005)



Variety of membrane shapes …

… that are reproduced by generic continuum models

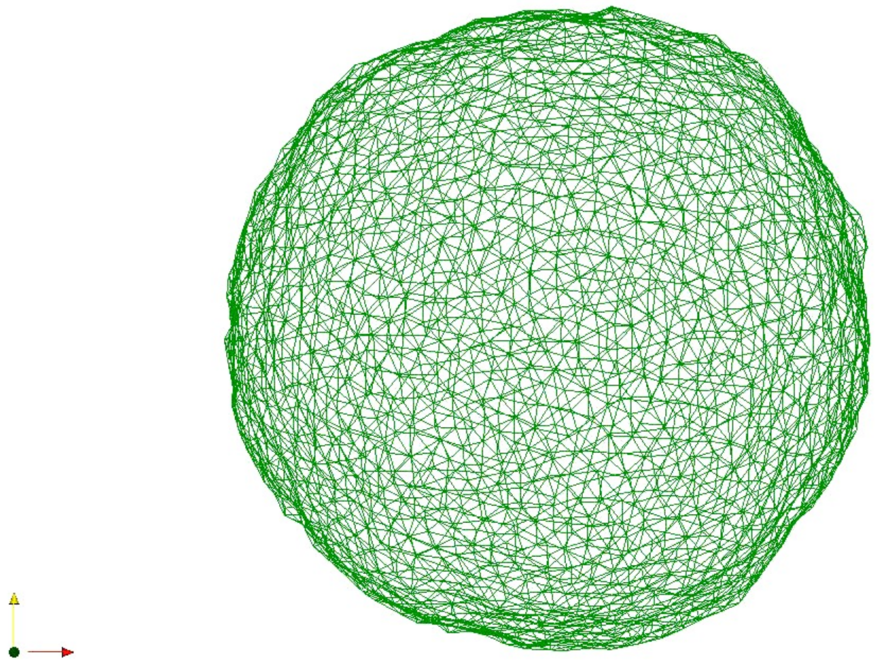


Hiroshi Noguchi et al
(2015)

⇒ Goal: See how much such models can tell us about tubular membrane structures

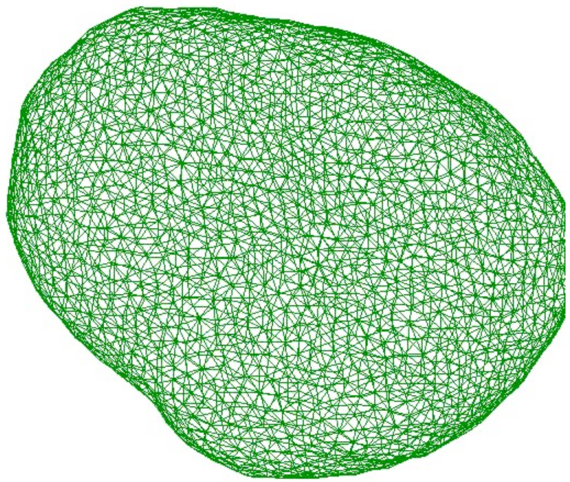
Example 1: Force free vesicle

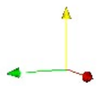
Fixed enclosed volume



Example 2: Force applied at one end

Fixed enclosed volume

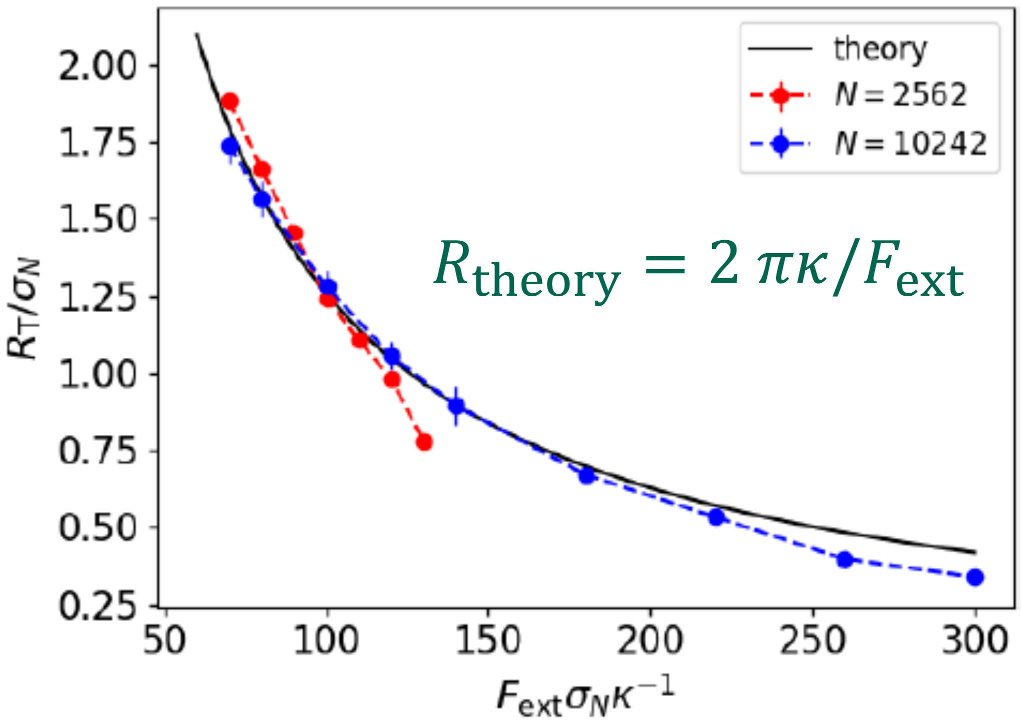


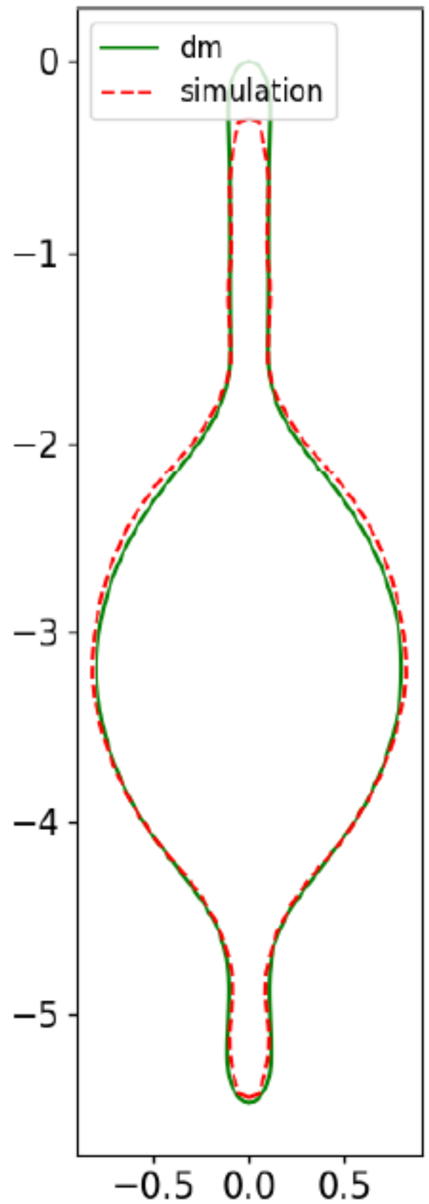


Numerical validation

For special symmetries, the Helfrich energy can be minimized semi-analytically

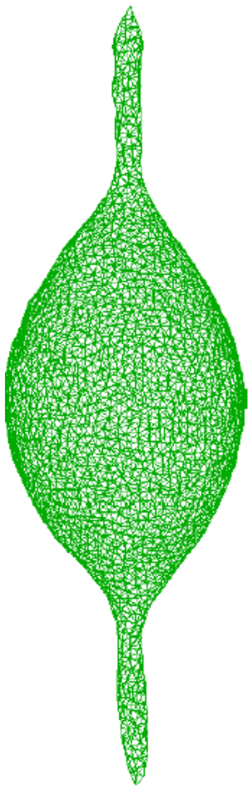
Tube radius vs. force



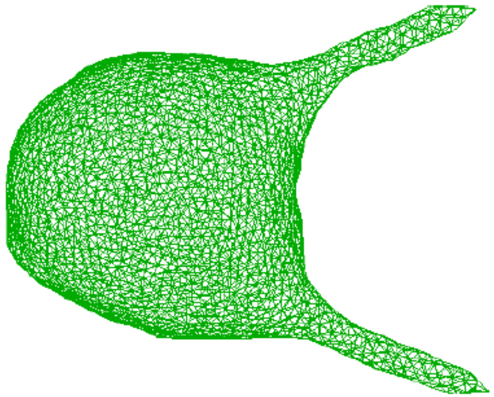


Interaction between tubes

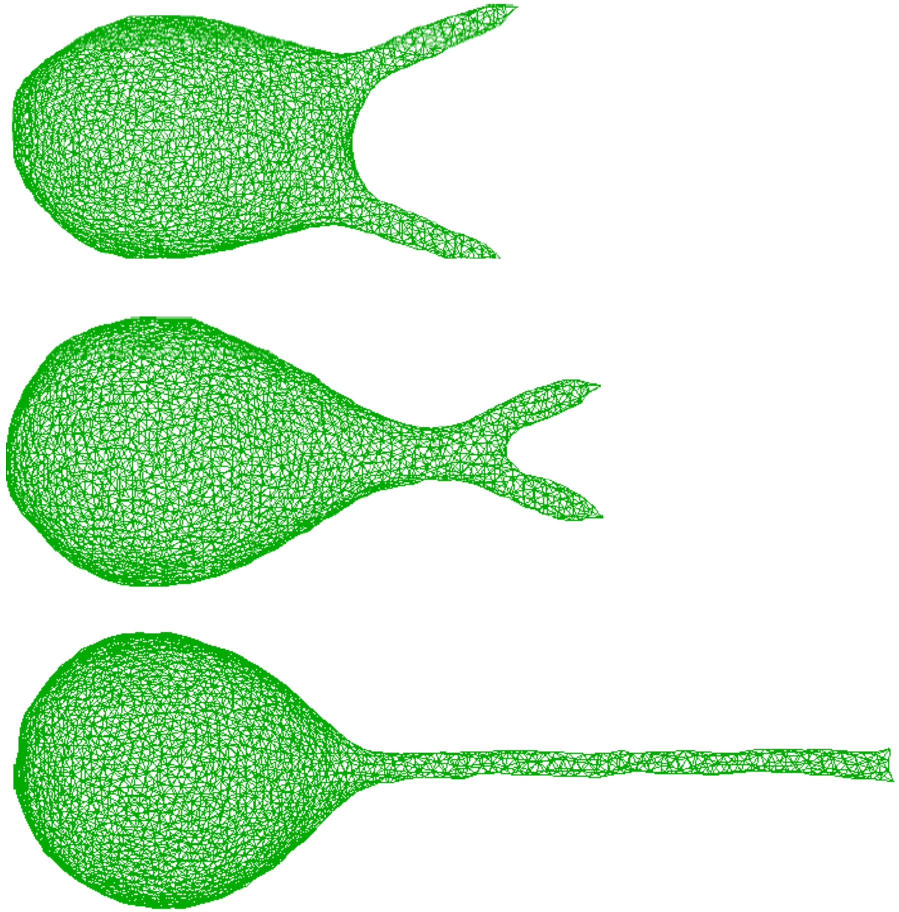
Initial



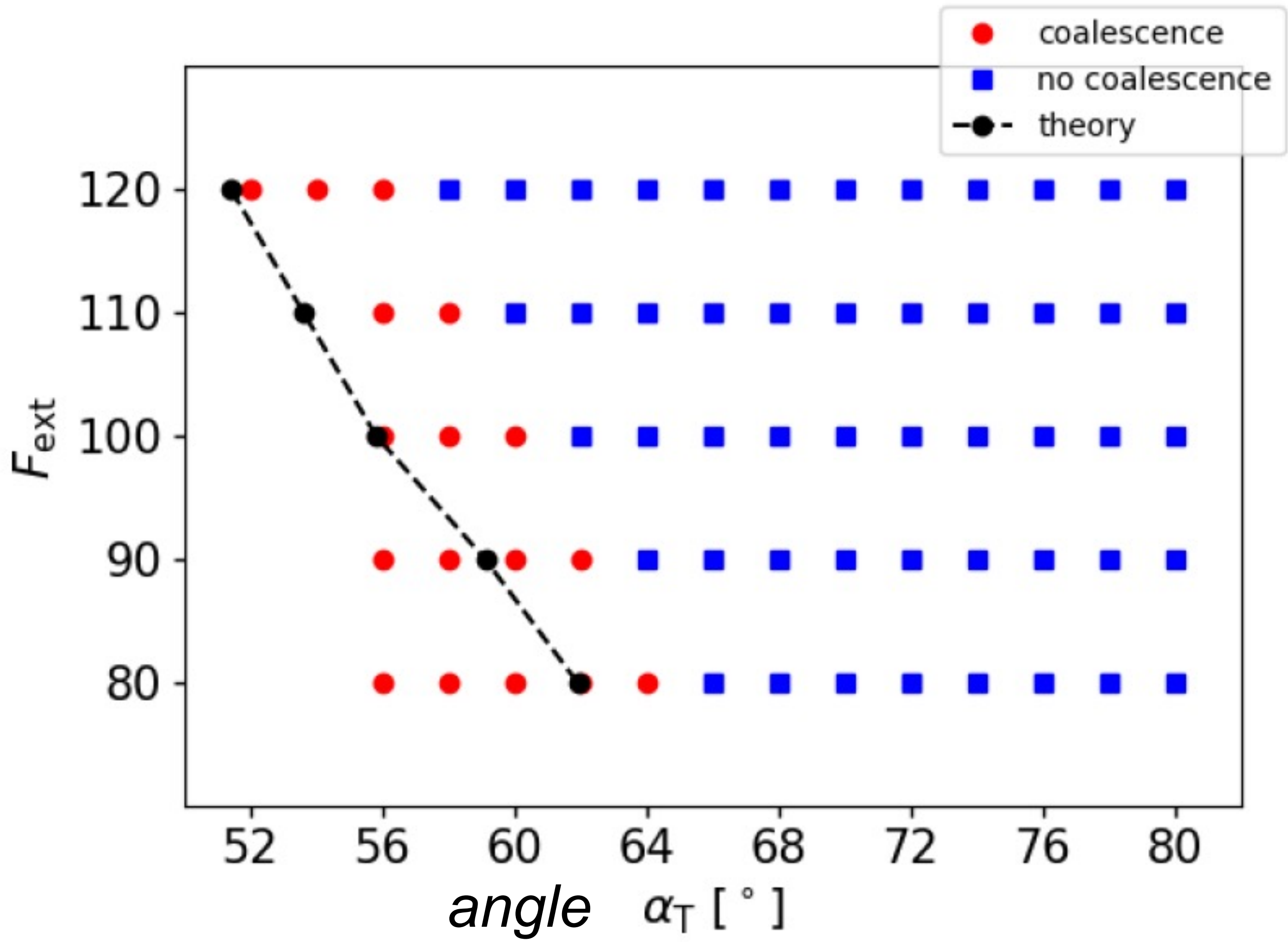
Reduce angle



Reduce angle further



Tube interactions: Onset of coalescence

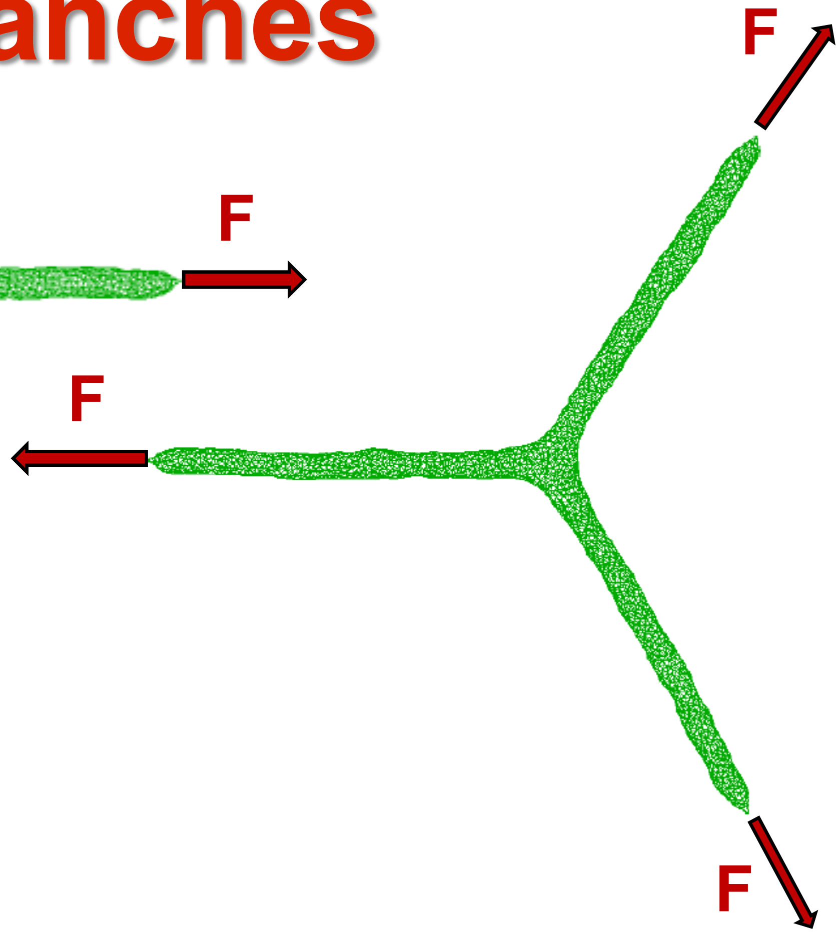


Theory

Cuvellier et al, Bioph. J. 2005

$$\alpha_T \approx \sqrt{\frac{R_T}{R_V\left(1+\frac{R_V}{L_T}\right)}}$$

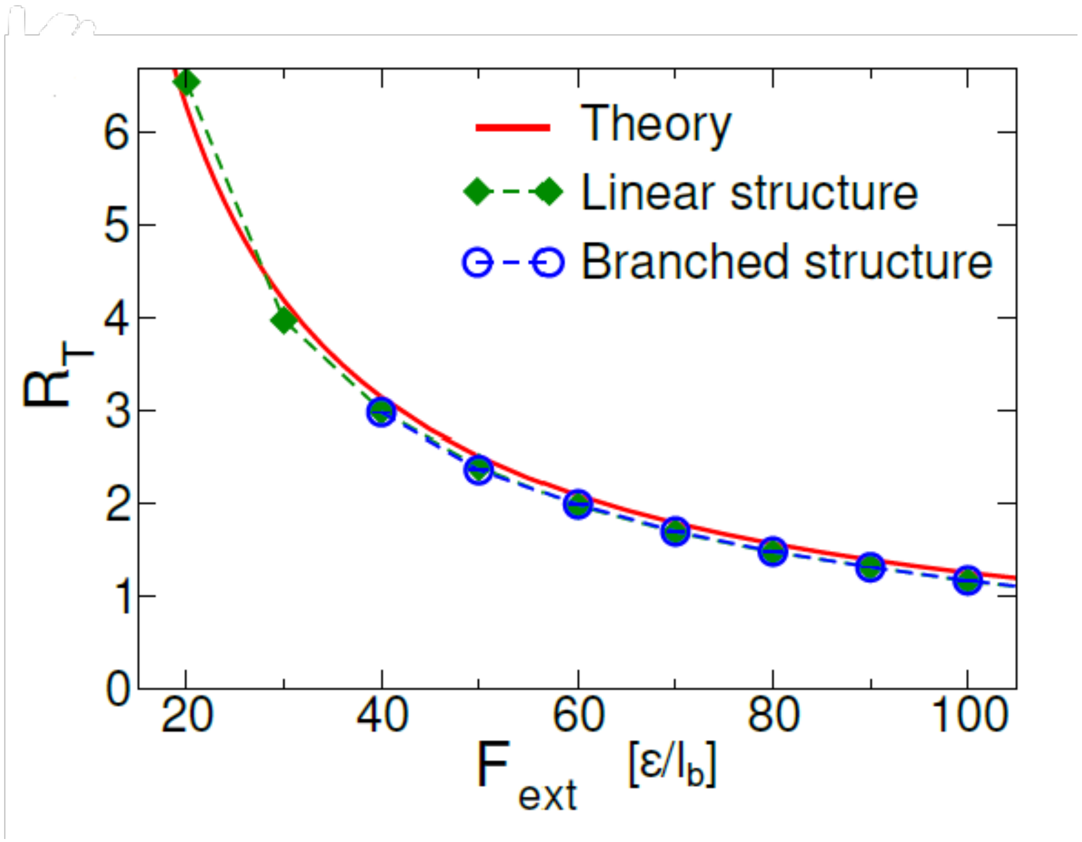
Tubes and Branches



Simplification: No attached vesicle
Enclosed volume not fixed

→ Focus on tubes
→ and, possibly, junctions

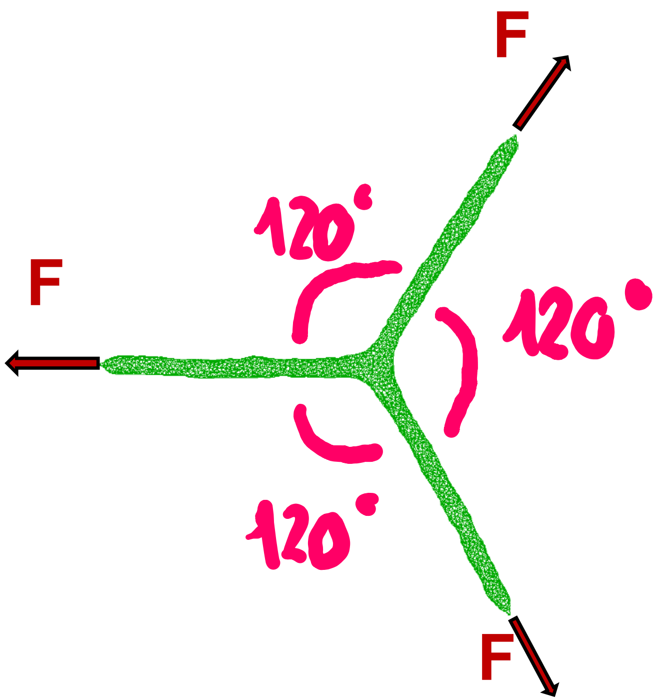
Tube radius

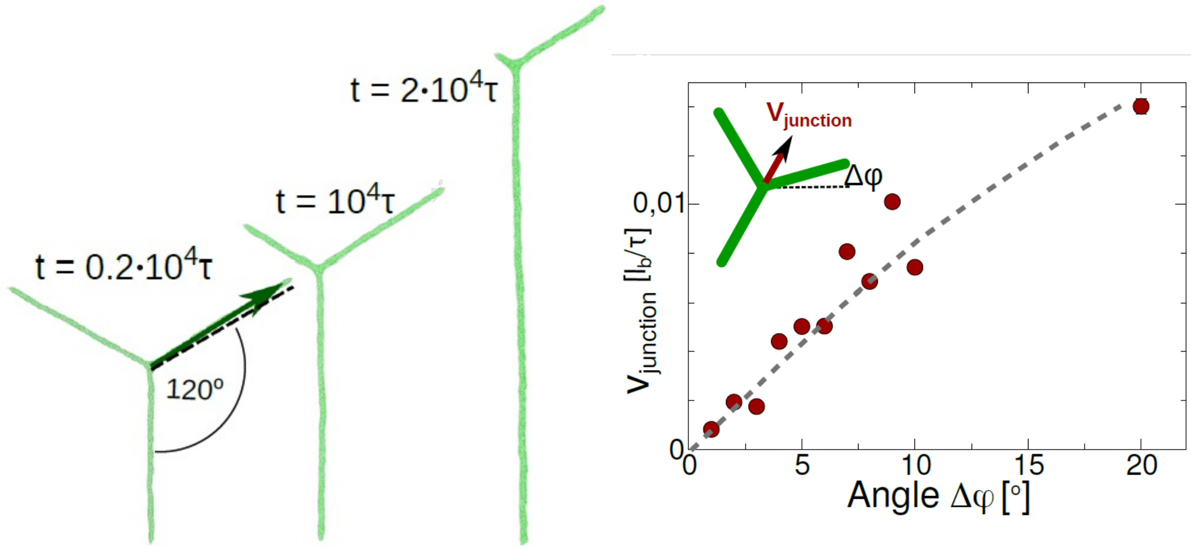


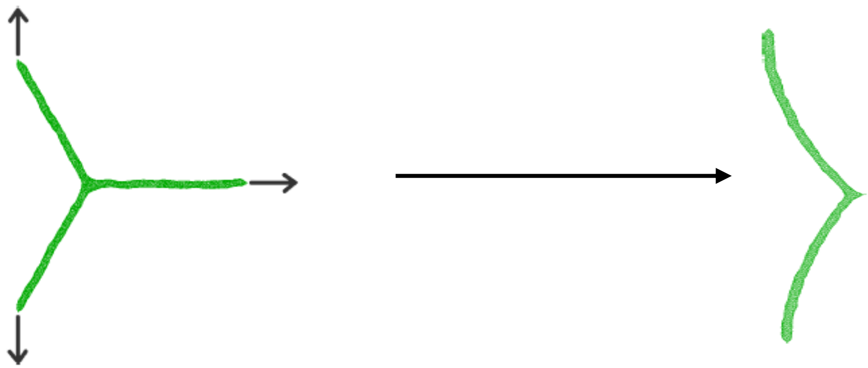
→ **Comparable for linear and branched structures**

Question 1: Angles at branch points ?

Observation: Only **one** possible stable angle: **120°**



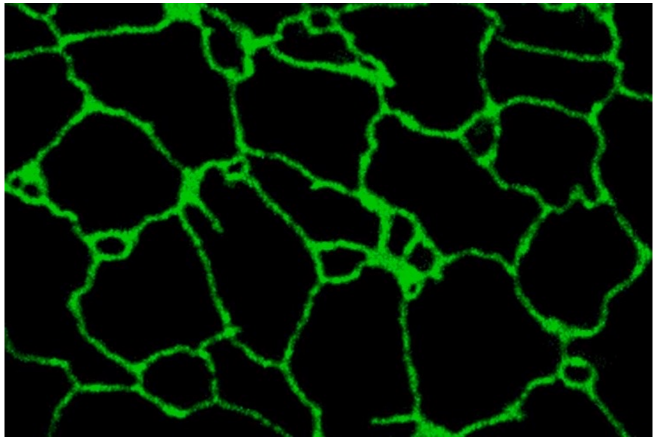




Comparison with experimental networks

Experiments: All angles close to **120°** √

Endoplasmatic reticulum



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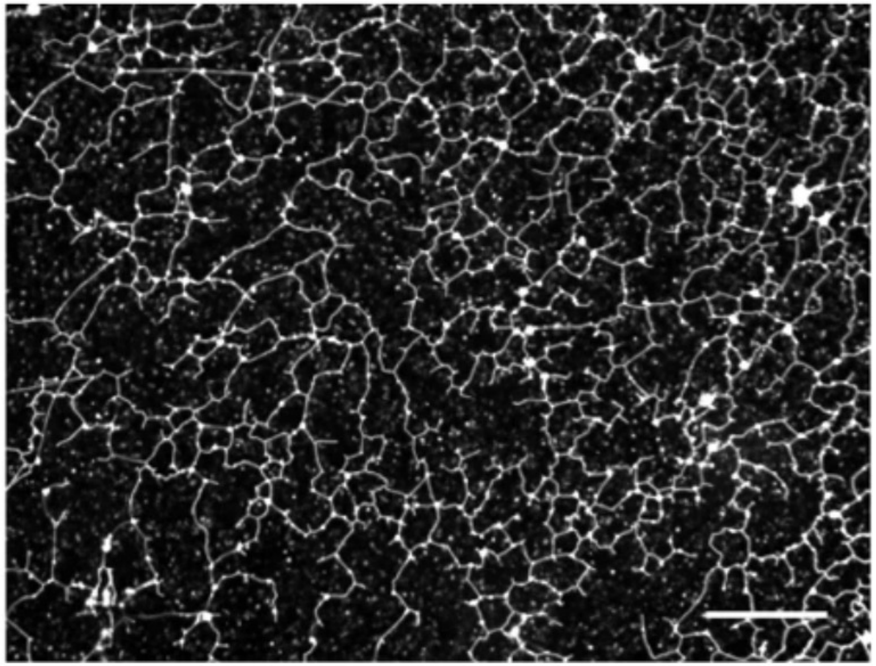
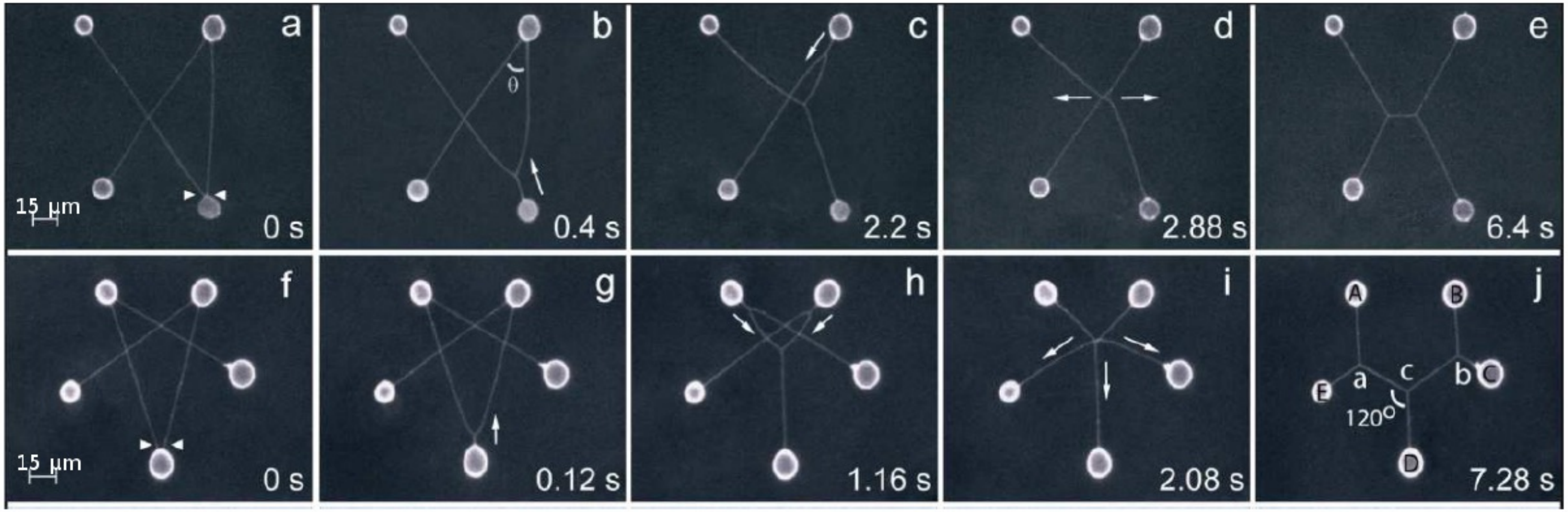
Reconstituted network



Powers, Wang, Liu, Rapoport Nature 543, 257 (2017)

Comparison with experimental networks

Time evolution of a liposome network

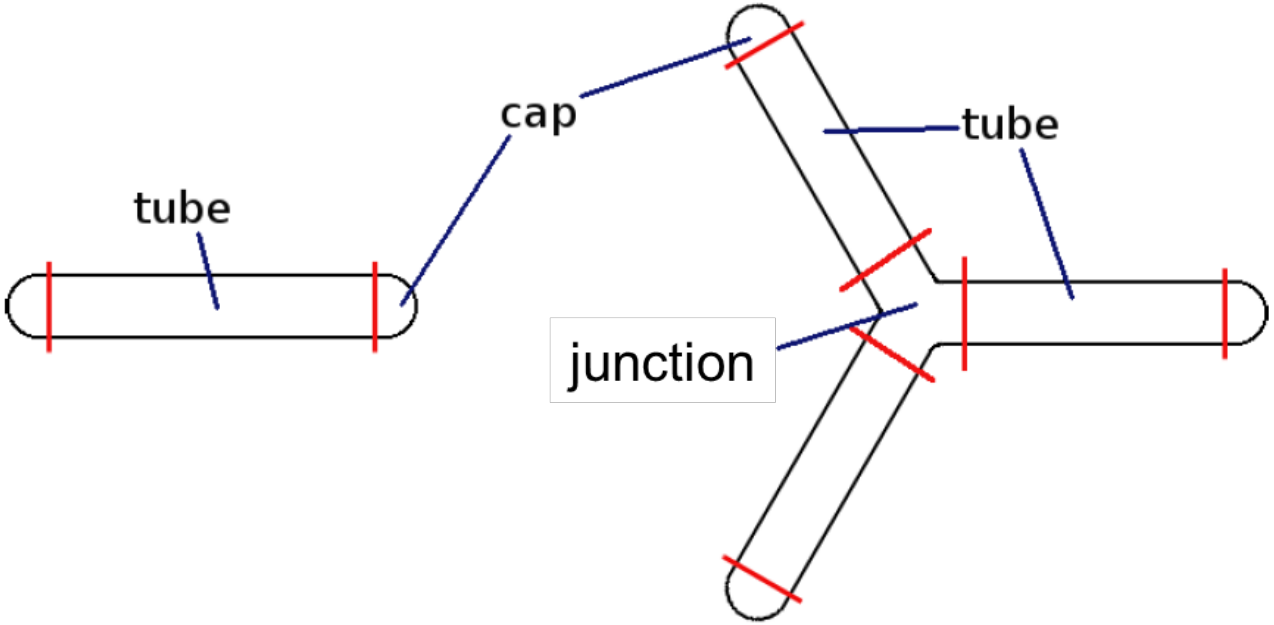


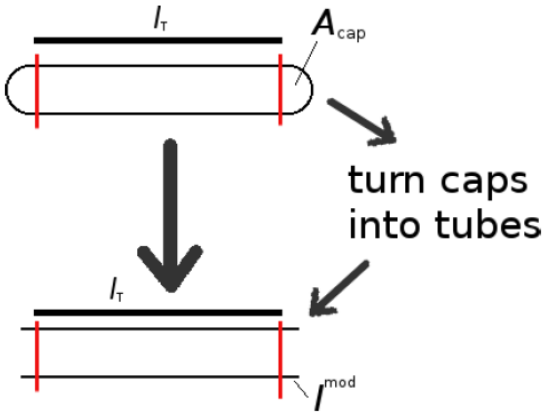
Lobovkina et al, Eur. Phys. J. E 254, 74 (2008).

Junctions move around, until all branch points reach 120°

2) Energy penalty for creating a branch

Analysis

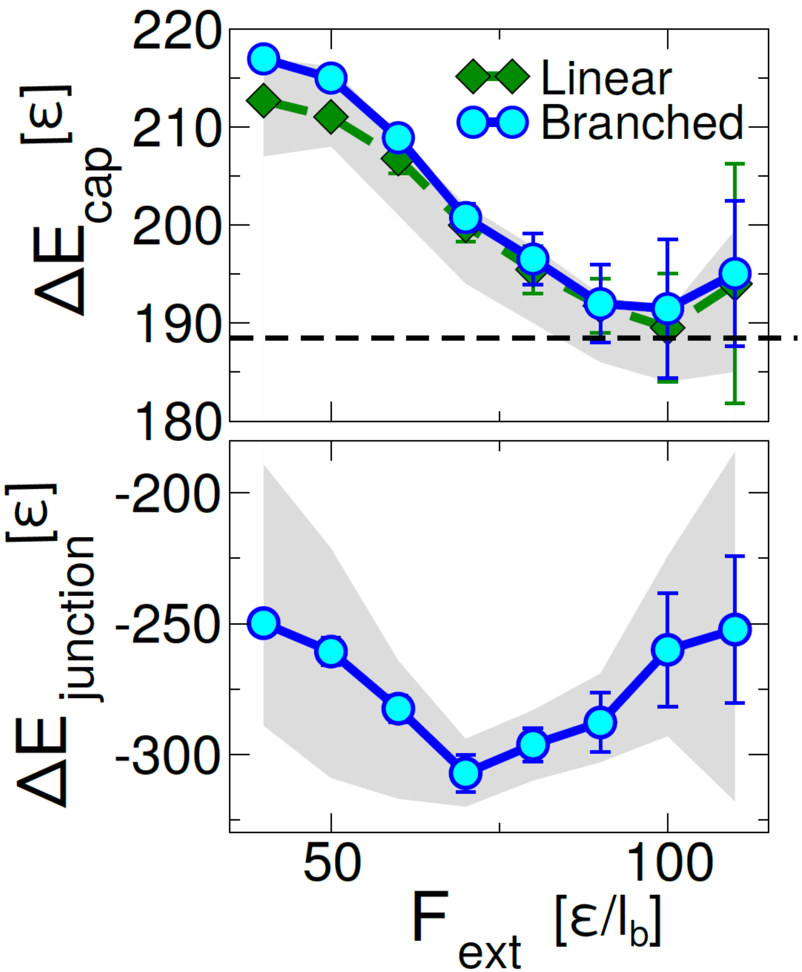




Cap/branch energy:

Energy difference between caps / branches and straight tubes with same membrane area

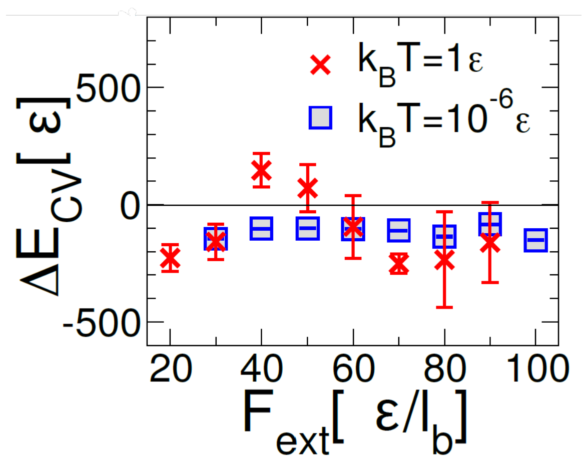
2) Energy penalty for creating a branch



⇒ Caps cost energy

But: Junctions are favorable!

⇒ Net effect: **No penalty!**
Even the energy of
Junction + cap is negative!



3) Are tubular structures stable?

Bahrami et al: **Tubes** can be stabilized without applying a force by fixing enclosed volume *(Bahrami, Hummer, ACS Nano 11, 9558, 2017)*

Our results:

3) Are tubular structures stable?

Bahrami et al: **Tubes** can be stabilized without applying a force by fixing enclosed volume *(Bahrami, Hummer, ACS Nano 11, 9558, 2017)*

Our results:

Thick tube

Thin tube

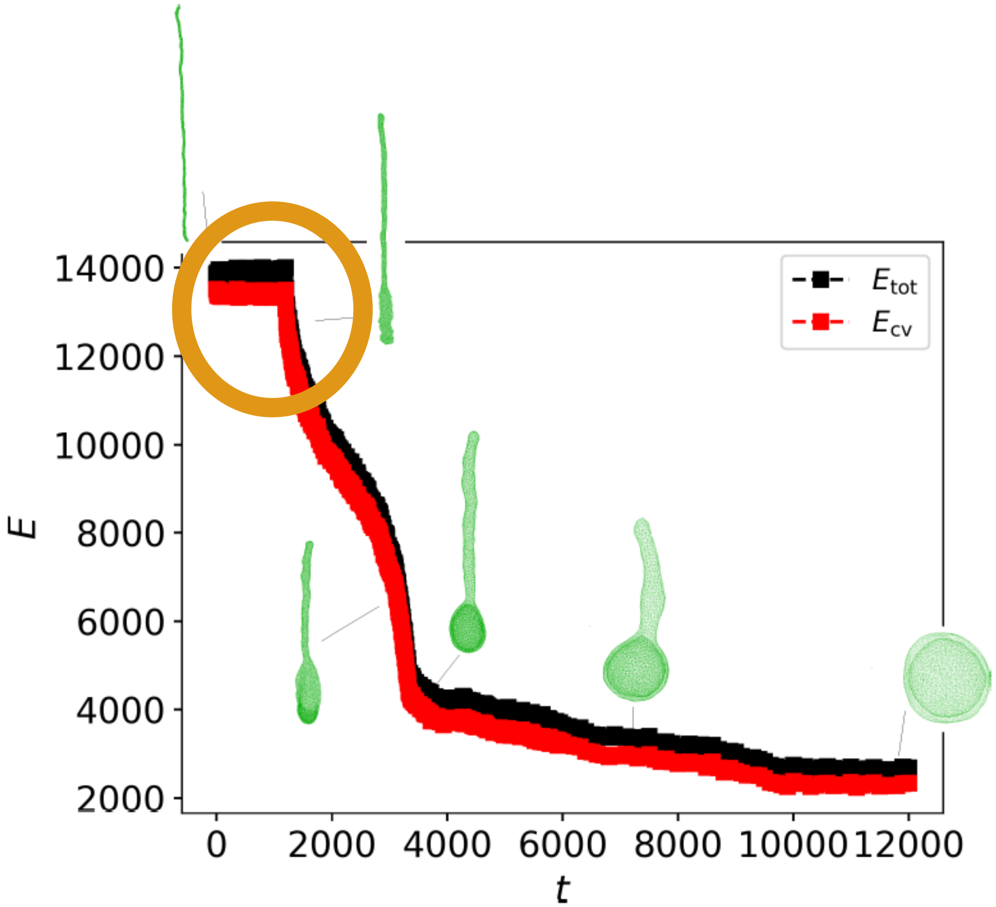
3) Are tubular structures stable?

Bahrami et al: **Tubes** can be stabilized without applying force by fixing enclosed volume *(Bahrami, Hummer, ACS Nano 11, 9558, 2017)*

Our results:

Thin tubes turn into double-wall vesicles after a long time (**activated** process)

Thicker tubes remain metastable



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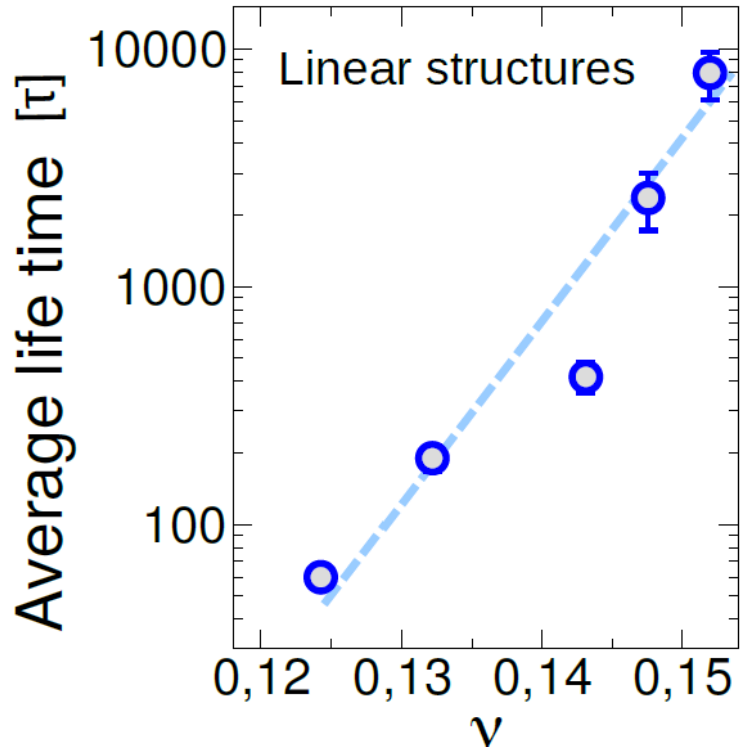
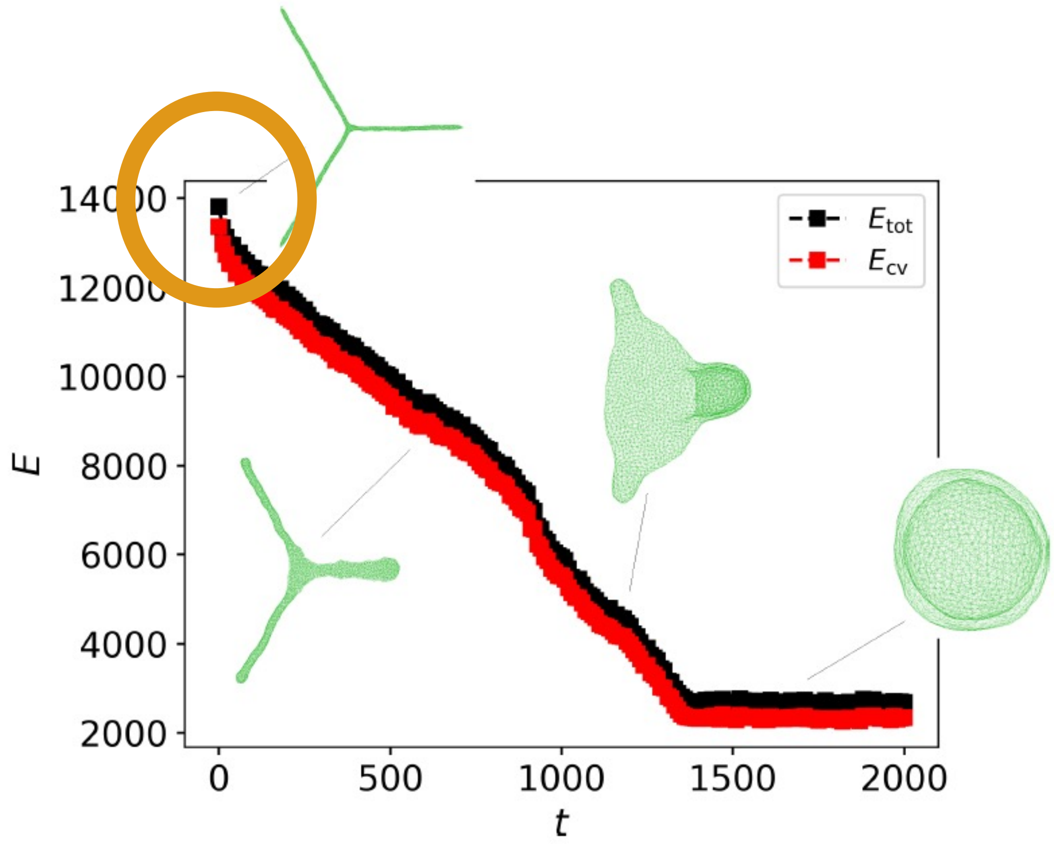


Reduced volume

3) Are tubular structures stable?

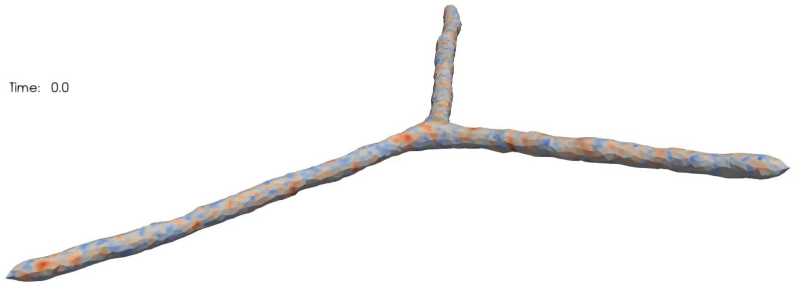
All branched structures transform **immediately** into double-walled vesicles



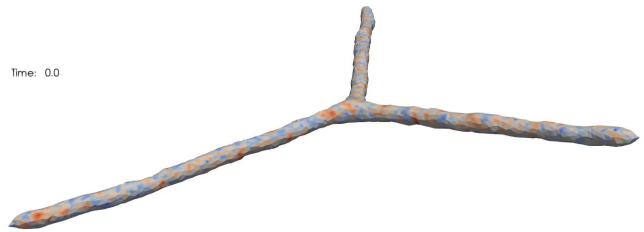
Spontaneous transition, no activation barrier

3) Are tubular structures stable?

Thick tubes

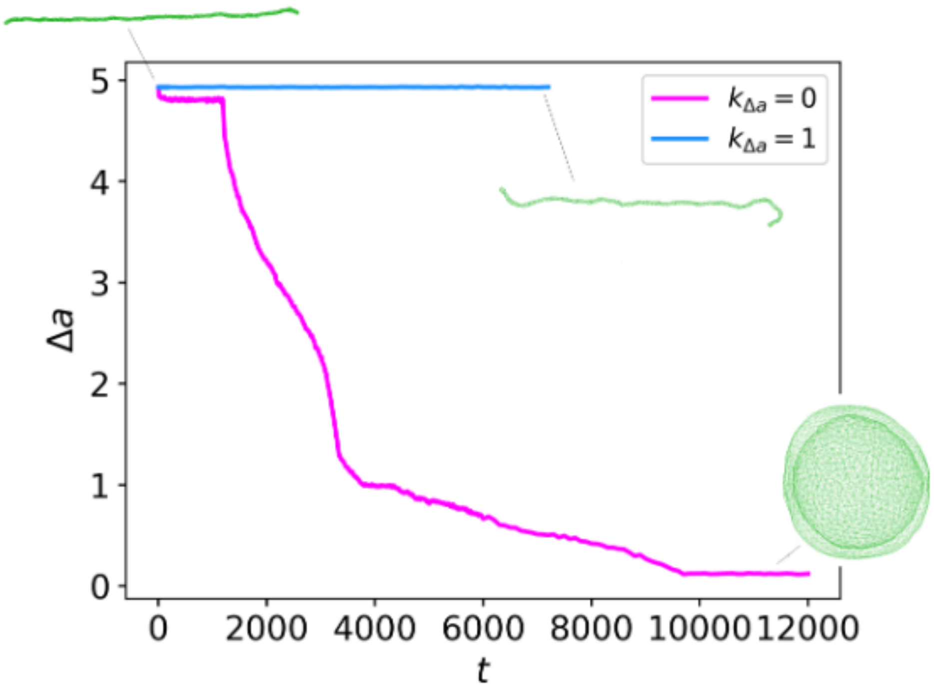


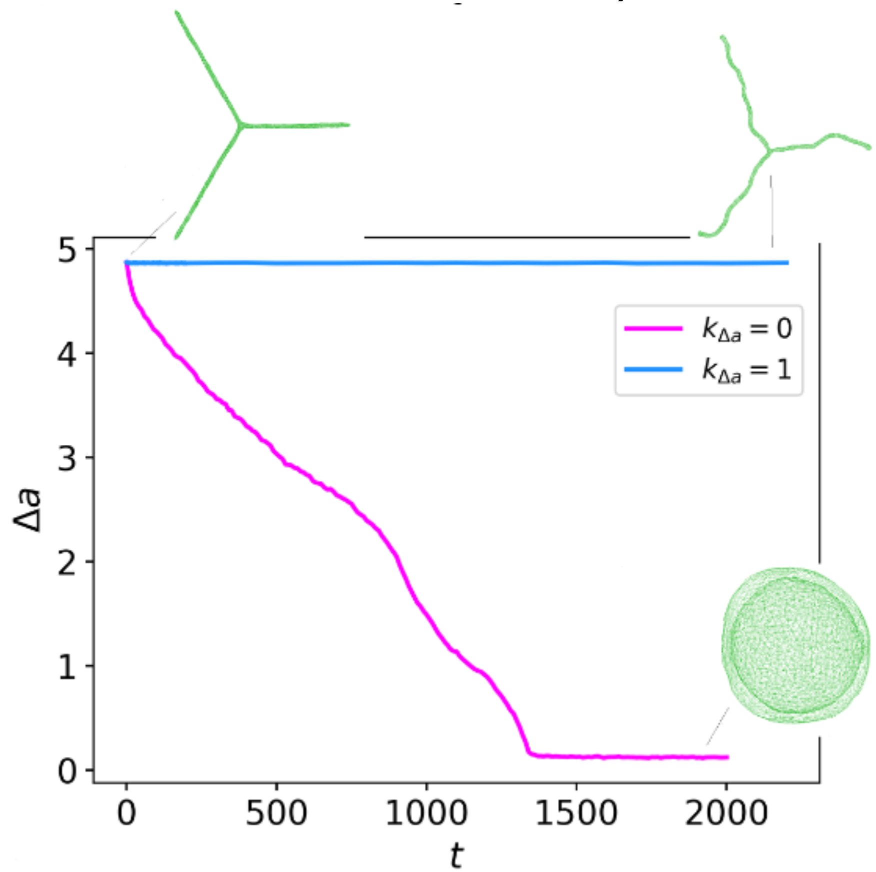
Thin tubes



3b) Can tubular structures be stabilized?

Next attempt: Additionally fix **mean curvature**
(“area difference” Δa between inner and outer leaflet)

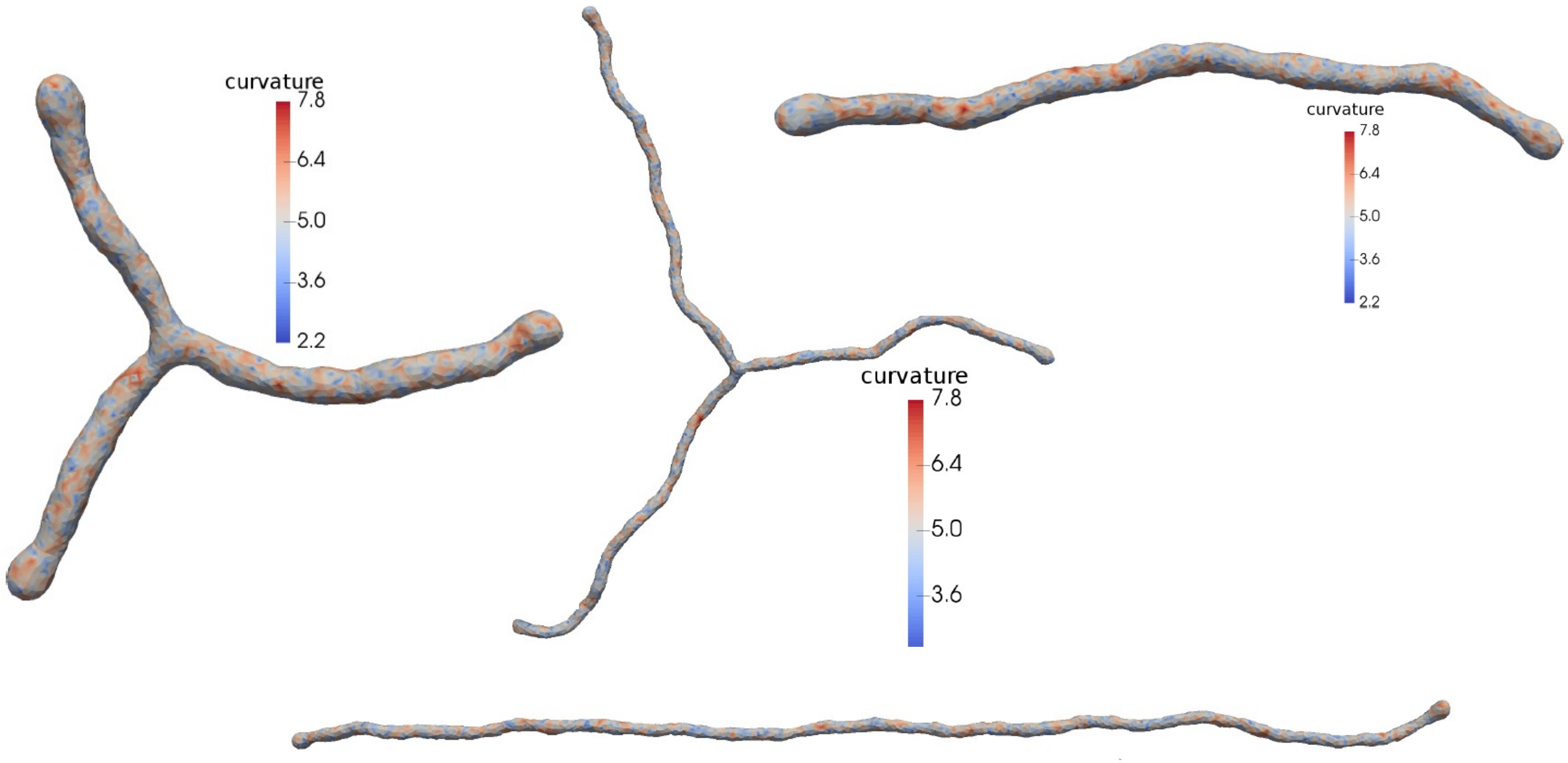




⇒ Both tubes and branches can be stabilized

3) Can tubular structures be stabilized?

Stable structures at fixed **mean curvature** (fixed Δa)

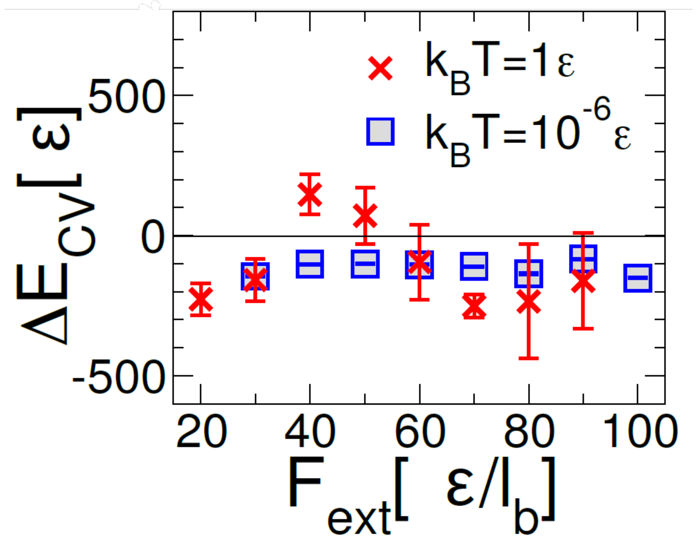


$\Rightarrow$ Both tubes and branches, thick and thin, are stabilized !

4) How about energy costs of branches ?

Recall force-driven structure:

⇒ Energy for creating a branch was negative!



Force free structure at fixed mean curvature Δa

⇒ Adding a junction has to be compensated by tube thinning

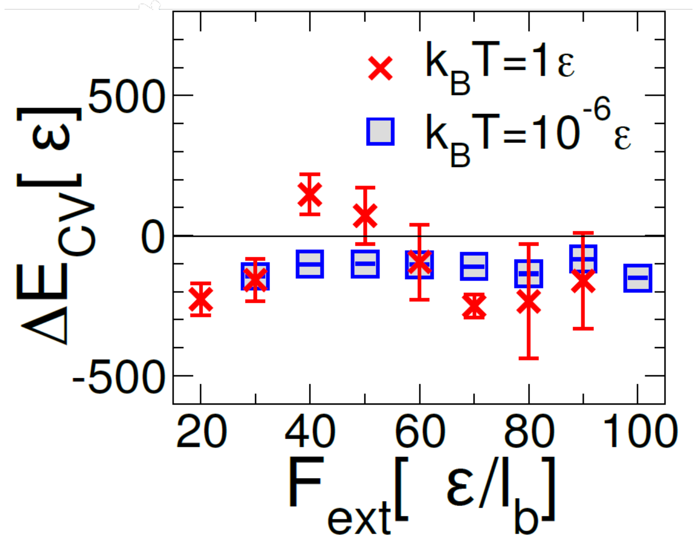
⇒ Net energy cost is positive!

$$\Delta E_{\mathrm{CV}} \approx \pi\kappa + \left|\alpha\, \Delta E_{\mathrm{junction}}\right| > 0$$

Fixed	Structure	E_{CV}/ϵ	ν	Δa			
–	Linear	9333 ± 26	0.186 ± 0.001	3.90 ± 0.01			
	Branched	9082 ± 34	0.193 ± 0.001	3.81 ± 0.01			
		C1 (Linear)			C2 (Branched)		
		E_{CV}	ν	Δa	E_{CV}	ν	Δa
Δa	Linear	9333 ± 3	0.186	3.90	8975 ± 3	0.191	3.81
	Branched	9470 ± 3	0.187	3.90	9117 ± 3	0.192	3.81
ν	Linear	9355 ± 3	0.186	3.91	8882 ± 3	0.192	3.79
	Branch	9538 ± 4	0.186	3.92	9079 ± 4	0.193	3.80
$\nu, \Delta a$	Linear	9342 ± 3	0.186	3.90	8951 ± 3	0.192	3.81
	Branch	9480 ± 3	0.186	3.90	9126 ± 3	0.193	3.81

4) How about energy costs of branches ?

Recall force-driven structure:
⇒ Energy for creating
a branch was negative!



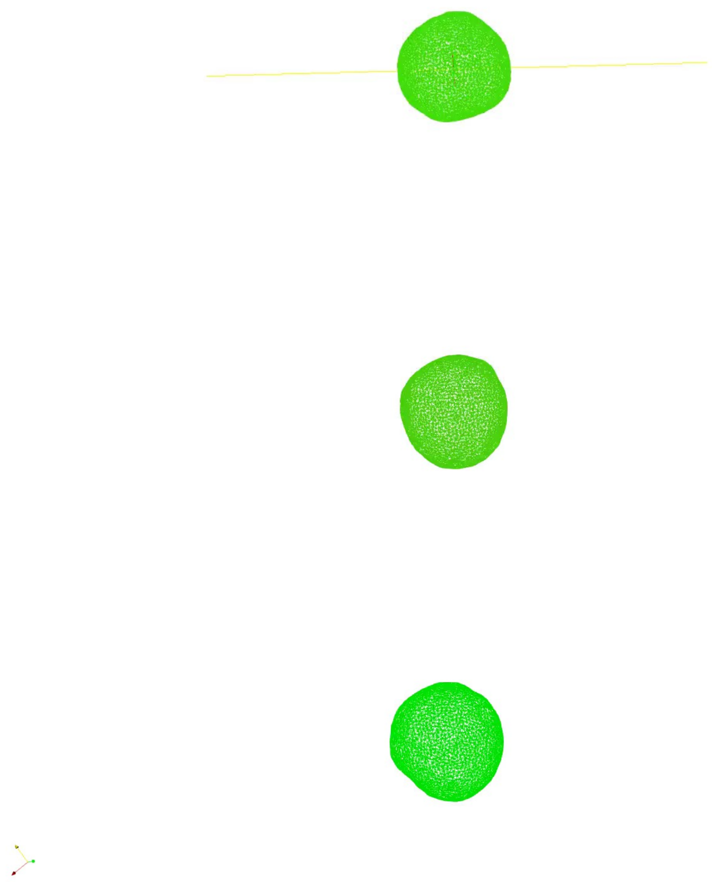
Force free structure at
fixed mean curvature Δa
⇒ Adding a junction has
to be compensated
by tube thinning

⇒ Net energy cost is positive!

$$\Delta E_{\mathrm{CV}} \approx \pi\kappa + |\alpha\, \Delta E_{\mathrm{junction}}| > 0$$

⇒ **Global effect!**
Core energy of junction
defect is negative!

5) Do stable four-fold junctions exist?



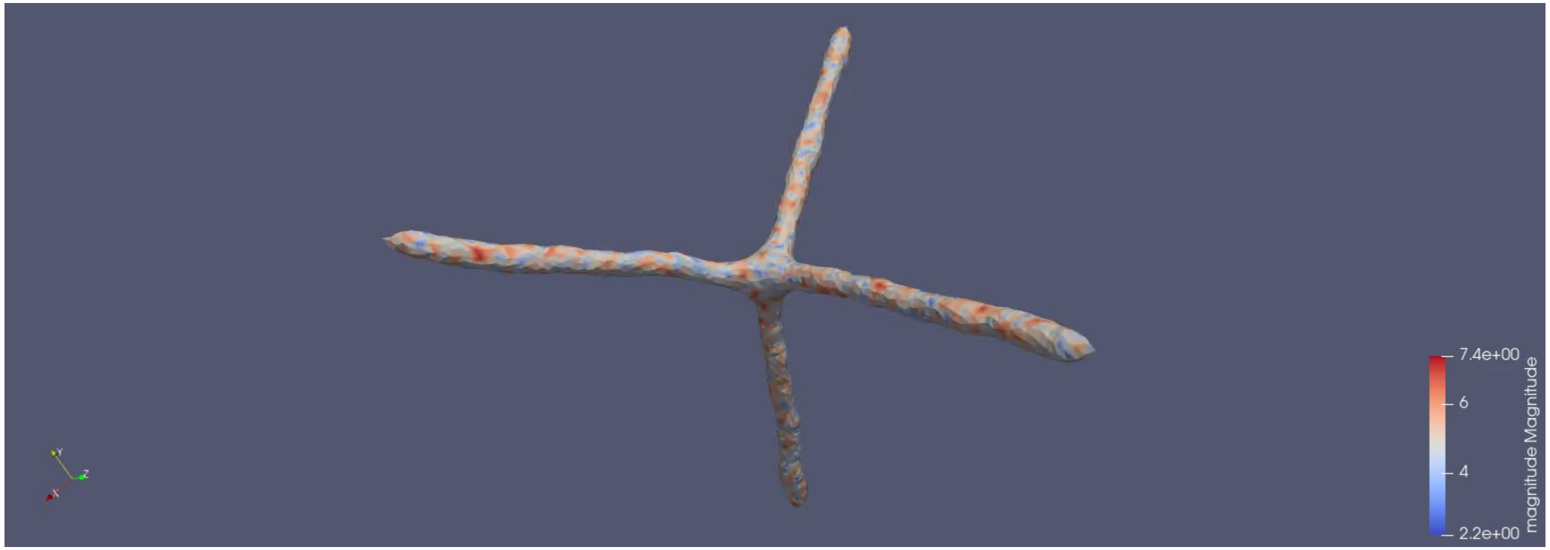
Force-driven structures:

⇒ Only tetrahedral junctions are stable.

⇒ All others break up into two threefold junctions

5) Do stable four-fold junctions exist?

Force-free structure with fixed Δa



$\Rightarrow$ In the absence of force, four-fold junctions break up into two three-fold junctions

Summary

Linear and branched structures can be stabilized in generic membrane models by imposing a few very simple constraints.

Simulations of generic models can give insights

- … why three-fold junctions with angle 180 degrees dominate.
- … why branched structures are abundant in nature: Junctions are locally stable. Eliminating them is only favorable if the entire tube network rearranges

(M. Jung, G. Jung, FS, Phys. Rev. Lett. 130, 148401, 2023)

Acknowledgments

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Enrico Schleiff (Frankfurt)

DYNAMEM

DFG Deutsche Forschungsgemeinschaft

TRR 146

MOGON

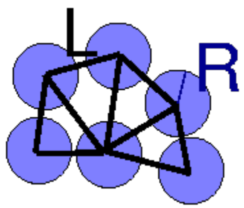
Simulation of elastic membranes I

Goal: Simulation of "self-avoiding" membrane models that are directly based on an elastic model for membranes

Example: Helfrich model (total curvature term only)

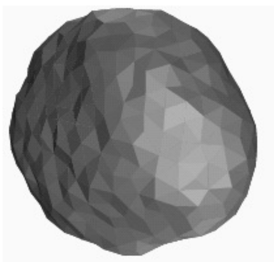
$$F = \int \mathrm{d}\mathbf{A} \left\{ \frac{\kappa}{2} K^2 \right\}$$

Realization: Triangulated membrane



Bond length $R < L < 2\sqrt{3}R$

$\Rightarrow$ „Self-avoiding" sheets
Membranes cannot cross

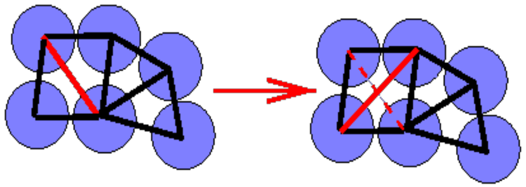


(Kantor et al, 1986, Ho, Baumgärtner, 1990, Kroll, Gompper, 1992)

Simulation of elastic membranes II

Membrane Fluidity: Dynamic triangulation

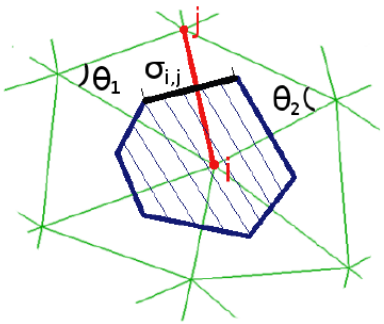
bond flip
moves



Membrane elasticity: Discretization of elastic free energy
for the spontaneous curvature model:

$$F = \frac{\kappa}{2} \sum_{\text{triangles}} \frac{1}{\sigma_i} \left(\sum_{j(i)} \frac{\sigma_{ij}\, \boldsymbol{r}_{ij}}{r_{ij}} \right)^2$$

(Noguchi, Gompper, Phys. Rev. E 2005)



with σ_{ij} : bond length in dual lattice

$$\sigma_{ij} = r_{ij}(\cot(\theta_1) + \cot(\theta_2))/2$$

σ_i : cell area in dual lattice

$$\sigma_i = \frac{1}{4} \sum_{j(i)} \sigma_{ij}\, r_{ij}$$