Nonlinear vesicles dynamics

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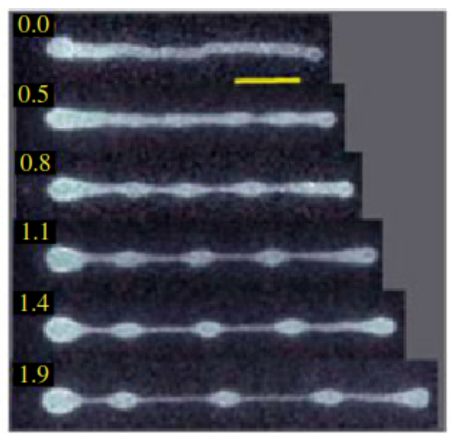
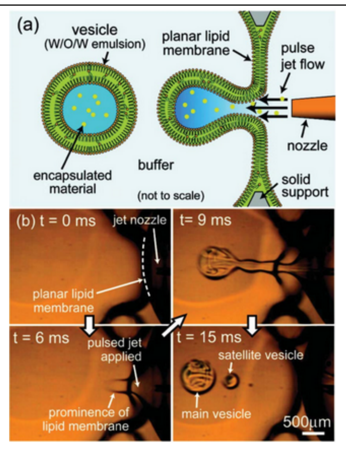
Introduction

Vesicles consisting of a two-layer membrane of amphiphilic lipid molecules are surprisingly flexible and at the same time slightly compressible surfaces. We study the evolution of vesicle shapes over time under various conditions. Our analysis of bilayer dynamics is based on a hydrodynamic approach, which treats a bilayer as an infinitely thin fluid layer on which shape-dependent forces applied to the surrounding viscous liquid are concentrated. The starting point of such consideration is the Helfrich energy [W.Helfrich, Z.Naturforsch (1973)]. Although we consider flows with low Reynolds numbers, which are governed by a linear hydrodynamic equation, the shape of the vesicle undergoes significant changes over time. This results in a highly nonlinear system of equations, necessitating the use of numerical simulation techniques to model the process. At first, we investigated the relaxation dynamics of vesicles. Specifically, normal modes were found, including the vicinity of bifurcation points. The bilayer is a "soft" object due to its small surface tension, and its shape can be easily deformed by external influences. In particular we model "pearling instability", induced by elongated forces, applied to the edges of prolate vesicles. We are also interested in processes in which a part of the membrane detaches from the main structure forming a vesicle. This kind of processes is important from biological point of view.



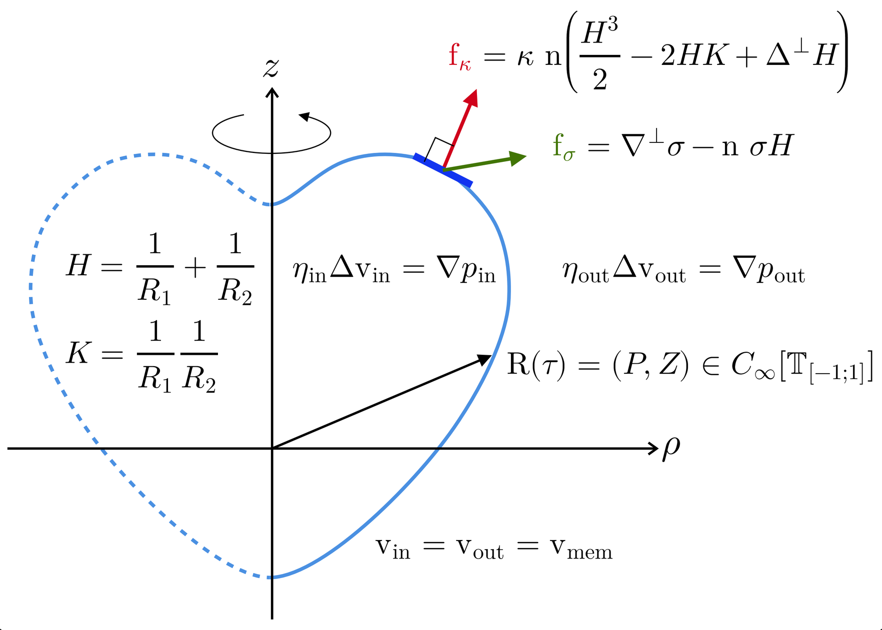
Tubular vesicle under pearling in elongation flow
Kantsler V., Segre E., Steinberg V. (2008)



Pulsed jetting, by Funakoshi et al. (2007):
(a) A schematic of the vesicle formation method.
(b) A sequence of images of vesicle formation captured by a high-speed camera.

Govering equation

Stokes flow, surface forces



$$f_\kappa = \kappa\, n\left(\frac{H^3}{2} - 2HK + \Delta^\perp H\right)$$

$$f_\sigma = \nabla^\perp \sigma - n\,\sigma H$$

$$H = \frac{1}{R_1} + \frac{1}{R_2} \qquad K = \frac{1}{R_1}\frac{1}{R_2}$$

$$\eta_{in}\Delta v_{in} = \nabla p_{in} \qquad \eta_{out}\Delta v_{out} = \nabla p_{out}$$

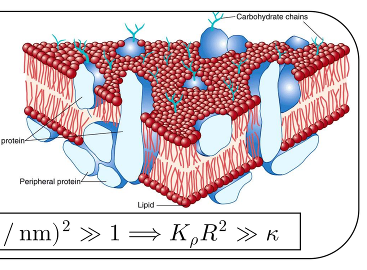
$$R(\tau) = (P, Z) \in C_\infty[\mathbb{T}_{[-1;1]}]$$

$$v_{in} = v_{out} = v_{mem}$$

Membrane energies

$$\mathcal{F}_\rho = \int \frac{K_\rho}{2}(n/n_0 - 1)^2 dS,\ K_\rho \sim 60\ \frac{k_B T}{\mathrm{nm}^2}$$

$$\mathcal{F}_\kappa = \frac{\kappa}{2}\int H^2 dS + \frac{\tilde\kappa}{2}\int K dS,\ \ \kappa \sim 20\ k_B T$$



$$\boxed{(R/\mathrm{nm})^2 \gg 1 \Longrightarrow K_\rho R^2 \gg \kappa}$$

Use Green function of Stocks equation to determine velocity, Integration along the polar angle was carried out analytically.

$$v = \int_{S_1} \widehat{G}(f_{\kappa 1} + f_{\sigma 1}) \rightarrow v_\mu = \int_\tau \widetilde{G}_{\mu\nu}\, f_\nu d\tau$$

Surface tension is 'fast' variable - adiabatic approach

$$\begin{cases} \partial_t n = -v\nabla n - n\nabla^\perp v \\ \sigma \approx -K_\rho(n/n_0 - 1) \end{cases} \Longrightarrow \partial_t \sigma = -v\nabla\sigma - \sigma\nabla^\perp v + K_\rho \nabla^\perp v$$

Linear nonlocal equation for σ

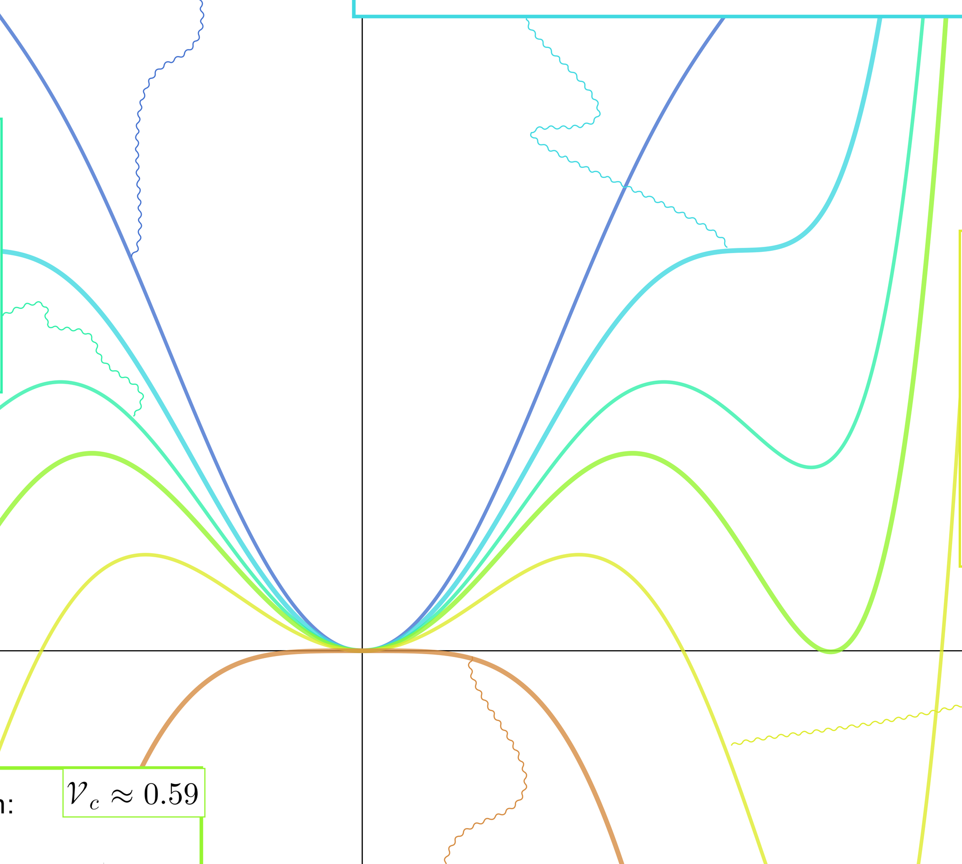
$$\boxed{\nabla^\perp v = 0} \Longrightarrow \int_{S_1}(\nabla^\perp \widehat{G})[\nabla_1^\perp - n_1 H_1]\sigma_1 = -\int_{S_1}(\nabla^\perp\widehat{G}) f_{\kappa 1}$$

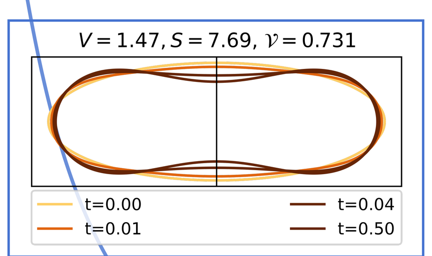
Energies are scaled by κ, surface tension σ by κ/R_0, velocity by $\kappa/\eta R_0^2$, time by $\eta R_0^3/\kappa$, where R_0 - appropriate lenght scale.

Final scheme $R \rightarrow f_\kappa \rightarrow v_\kappa \rightarrow \nabla^\perp v_\kappa \rightarrow \sigma \rightarrow v_\sigma \rightarrow \partial_t R$

Flattened branch on schematic bifurcation diagram

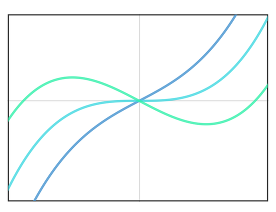
Conservation of volume and surface area, thus describing by reduced volume $\boxed{\mathcal{V} = \frac{V/(4\pi/3)}{(S/4\pi)^{3/2}}}$





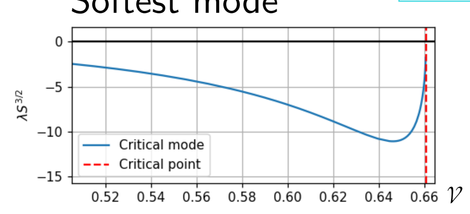
Saddle-Node Bifurcation

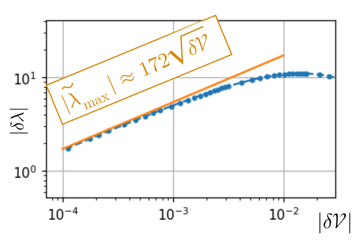
$\mathcal{V}_{sto} \approx 0.66$

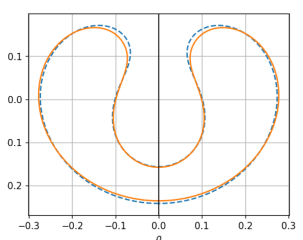


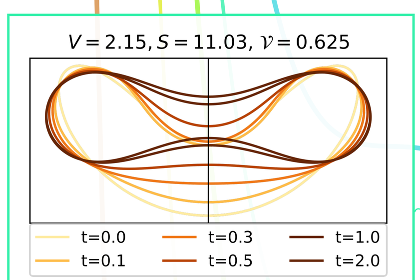
$$v = \frac{d(\delta x)}{dt} \approx \delta x^2 + \beta$$
$$\delta x_{eq} = \pm\sqrt{-\beta}$$
$$\partial_x v = 2\delta x \rightarrow \pm 2\sqrt{-\beta}$$

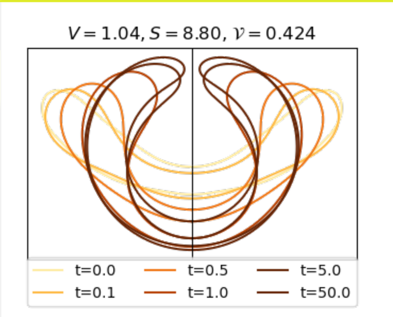
Softest mode





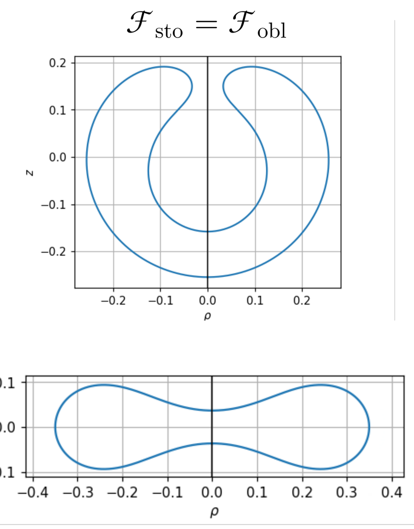






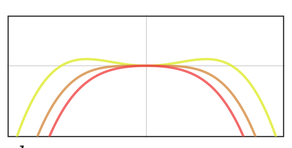
First order phase transition: $\mathcal{V}_c \approx 0.59$

$\mathcal{F}_{sto} = \mathcal{F}_{obl}$



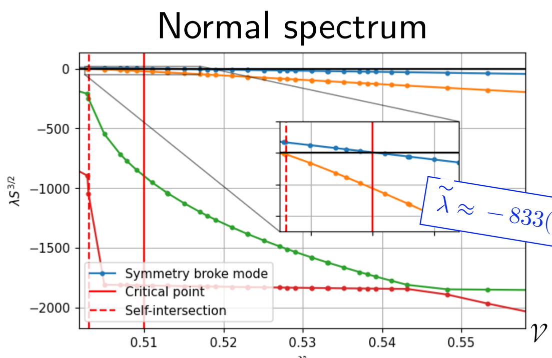
Supercritical Pitchfork Bifurcation

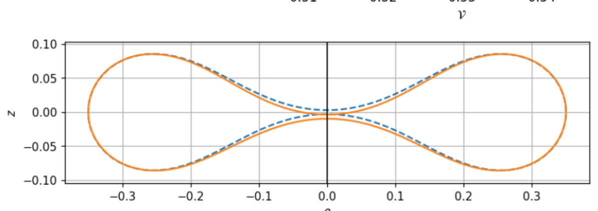
$\mathcal{V}_{ob} \approx 0.51$



$$\frac{dx}{dt} = v(x) = -\alpha x - x^3$$
$$\partial_x v = -\alpha$$

Normal spectrum





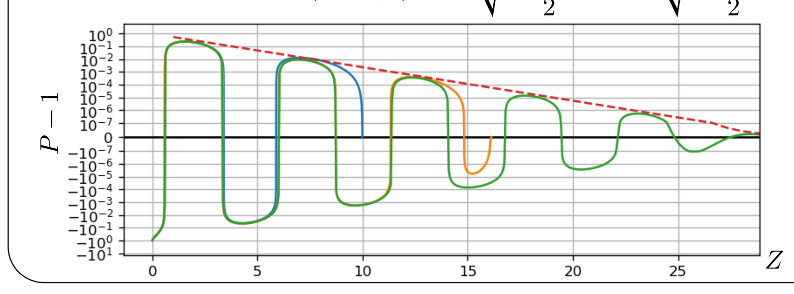
Asymptotic prolate shapes

Prolate vesicles have asymptotic shape: tube with universal edges:
It can be determined as solution of force balance equation,where equlubrium pressure and surface tension can be found using balance far away from edge and scale invariance of Helfric energy.

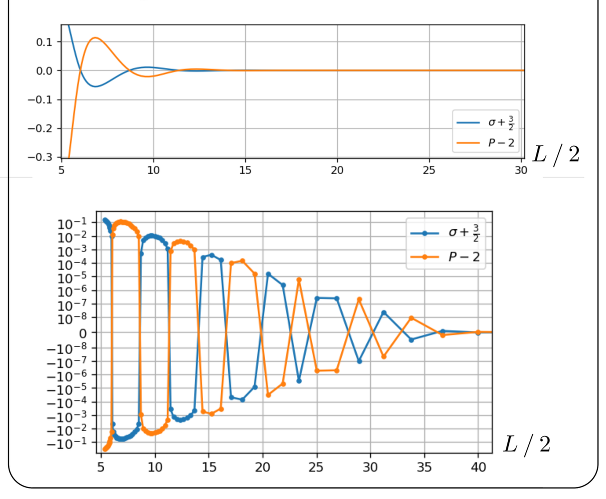
$$\begin{cases} \Delta P_{eq} = -\sigma_{eq}H + \kappa(H^3/2 - 2HK + \Delta^\perp H) \\ R \rightarrow R/\lambda \Longrightarrow \mathcal{F}_\kappa = \frac{\kappa}{2}\int H^2 dS \rightarrow \mathcal{F}_\kappa \end{cases} \Longrightarrow \boxed{\sigma_{eq} = -\frac{3}{2},\ \Delta P_{eq} = 2}$$

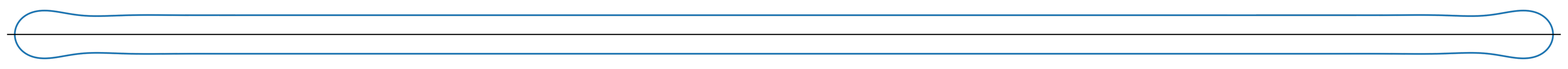
Far away from edge asymptotic:

$$P - 1 = \delta P \propto A e^{-\varkappa z}\sin(kz + \phi_0),\ \varkappa = \sqrt{\frac{\sqrt{3}-1}{2}},\ k = \sqrt{\frac{\sqrt{3}+1}{2}}$$



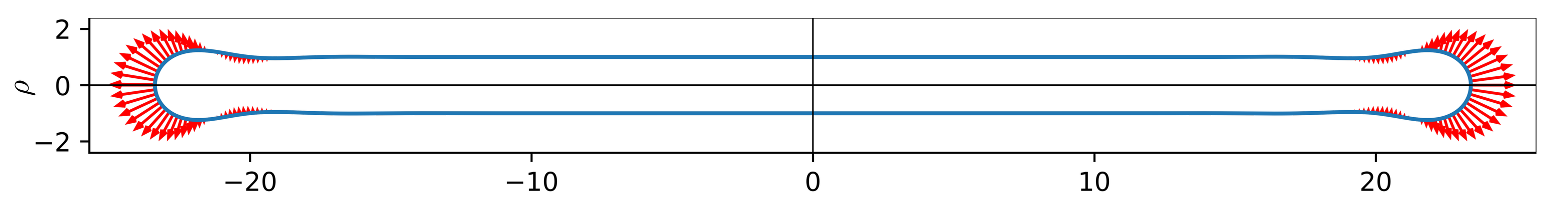
Convergence to the limit values





Pearling instability

Apply model normal elongating force $f = \gamma(H - H_0) \Longrightarrow$ same state is equlibrium with corrected surface tension $\delta\sigma = \gamma$

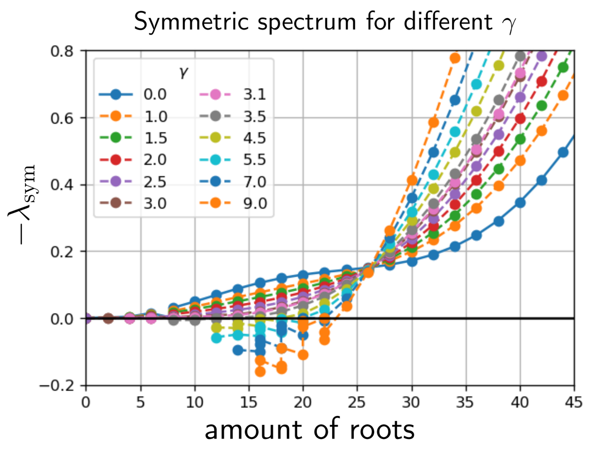


Linear stability theory

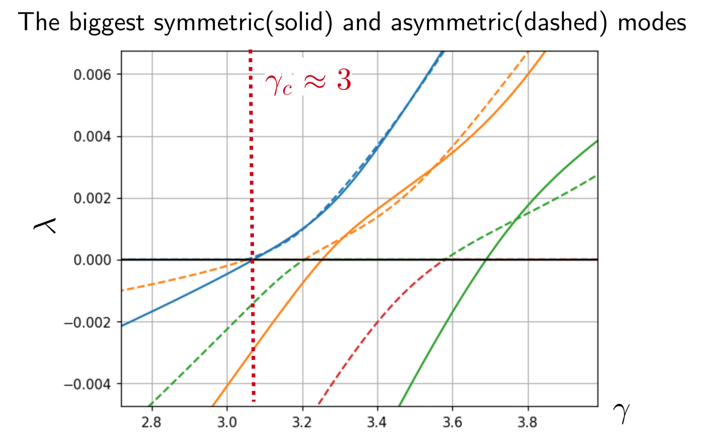
$$R = R_{eq} + \delta R(t) \quad \partial_t R = F[R] \Longrightarrow \partial_t \delta R = \frac{\delta F}{\delta R}\delta R = \widehat{\Lambda}\delta R$$

Find normal modes $\underline{\widehat{\Lambda}\delta N_k = \lambda_k \delta N_k}$ (Localy stable if $\forall k:\ \mathbb{R}\lambda_k < 0$)

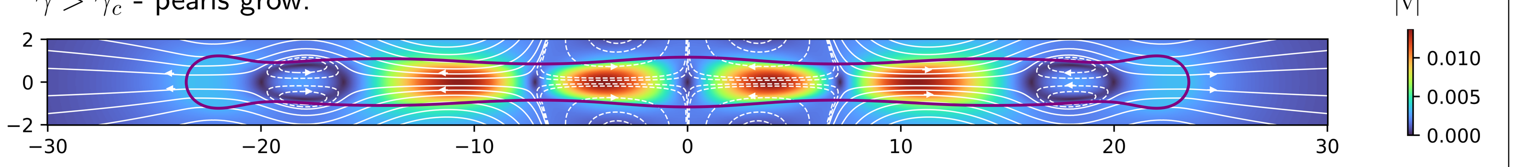
Symmetric spectrum for different γ



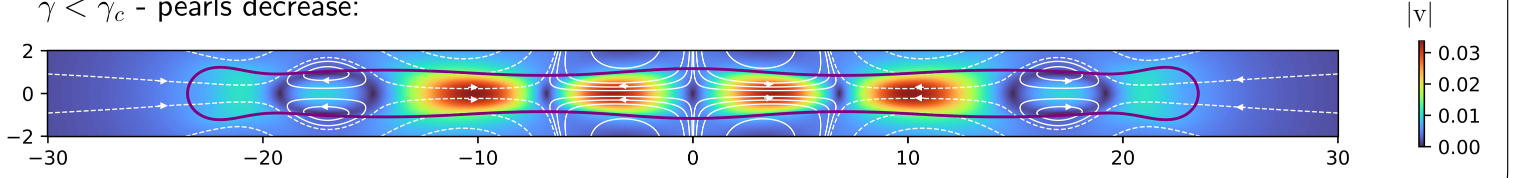
The biggest symmetric(solid) and asymmetric(dashed) modes



$\gamma > \gamma_c$ - pearls grow:

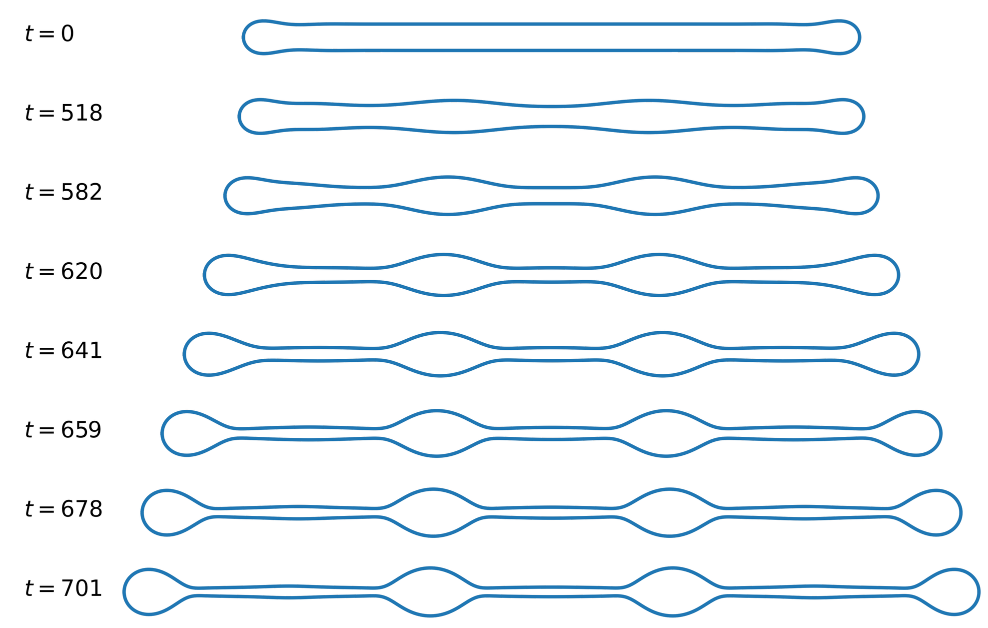


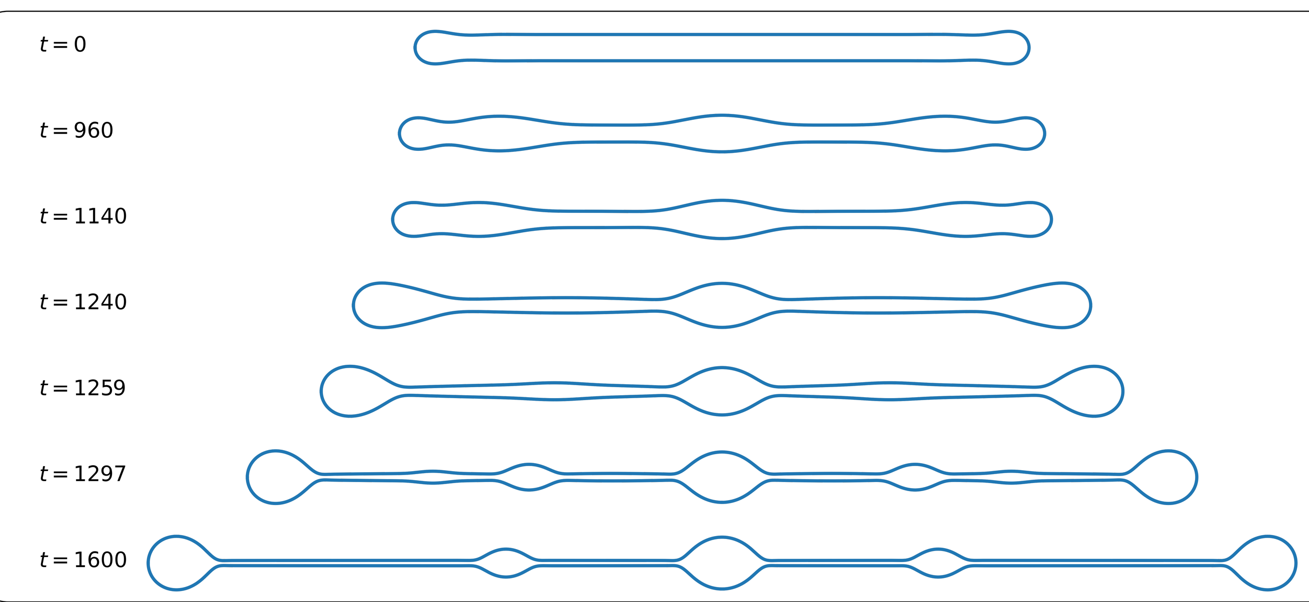
$\gamma < \gamma_c$ - pearls decrease:



*v is scaled by $\frac{\kappa}{\eta}\frac{1}{R_0^2}$

Development of the most unstable mode $(\delta R \sim 10^{-5})$





Conclusion

We developed a reliable algorithm for modeling the nonlinear dynamics of closed axially symmetric vesicles. We demonstrated relaxation dynamics to previously known stationary shapes. Critical parameters of bifurcation points were obtained for flattened vesicles. Asymptotic shape and equilibrium parameters for elongated vesicles were derived. The "pearling instability" under the action of tensile forces applied to the edges of the vesicle was considered;force critical values were obtained.
We simulated the development of instability at a supercritical force value in a nonlinear regime with "pearls" formation.

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