Mesoscale model for cavitation in lipid membranes

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Cavitation — formation of vapor bubbles in a liquid under tension — has catastrophic consequences when uncontrolled. At ambient temperature, pure water withstands extremely negative pressures (below $-100\,\mathrm{MPa}$ [1]) whereas at biological conditions, when contaminated, several events per day are observed. Recent molecular simulations suggested this drop in tensile resistance is due to lipid structures in the liquid [2]. However, being cavitation thermally activated, quantitative predictions on its occurrence inherit strong uncertainties from the exponential scaling with the activation energy. The challenge is further compounded by the different length and time scales involved, ranging from molecular agitation to hydrodynamics.

In this talk, we develop a mesoscale model of cavitation within lipid membranes that accounts for their elasticity while capturing the microscopic interactions between leaflets. By combining rare event techniques and fluctuating membrane dynamics with a diffuse description of leaflets [3,4,5], we compute activation energies, critical bubble configurations (as seen in Fig. 1), and corresponding diffusion coefficients. The predicted cavitation pressure is consistent with previous estimates. Our approach offers a versatile and computationally efficient way to connect the microscopic features of the lipid interface, such as composition, with the hydrodynamics of the nucleated bubble.

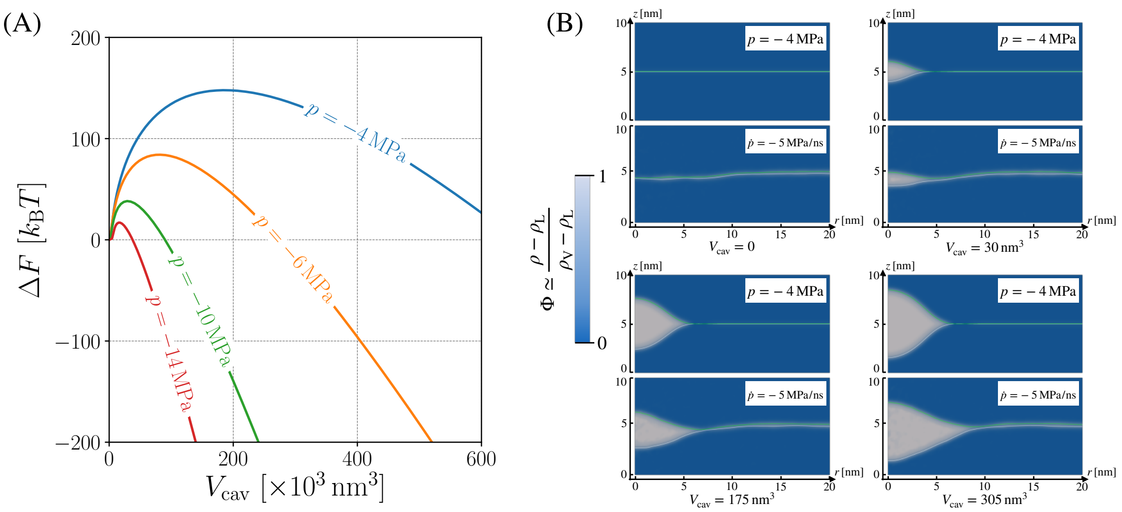

Figure 1: (*A*) Minimum free energy pathway (MEP) for cavitation under different negative pressures, parametrized by the cavity volume. (*B*) Slices of the cavitation evolution along the MEP, upper-half, compared to fluctuating membrane dynamics under decreasing pressure, lower-half. The contour plot shows the normalized vapor content while green and white lines represent lipid tails from upper and lower leaflets, respectively.

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[1] Magaletti et al., *Scientific Reports* **11**, 1-10 (2021)
[2] Kanduč et al., *PNAS* **117**, 10733-10739 (2020)
[3] Bottacchiari et al., *Communications Physics* **5**, 1-12 (2022)
[4] Bottacchiari et al., *PNAS Nexus* **3**, pgae300 (2024)
[5] Bussoletti et al., *Scientific Reports* **14**, (2024)