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Determining the Gaussian Curvature Modulus of Lipid Membranes in Simulations: A Comparative Study via Global Shape Transformations and Local Stress Distributions

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The Gaussian curvature modulus κ-bar matters for many important biological processes that involve topological and/or boundary changes of cell membrane, e.g. endo- and exo-cytosis. However, only sparse experimental measurements of have been reported, and even fewer accurate results obtained via computer simulations exist. Here, we propose a novel approach to determine κ-bar *in silico* by monitoring patch-closure processes of pre-curved circular bilayers. Applying this method to two different coarse-grained (CG) membrane models, namely the generic Cooke model [1] and the more finely-resolved and systematically parameterized MARTINI model [2], we find elastic ratios between the two curvature moduli, κ-bar/κ, in the range between −0.85 and −1.05, in line with previous estimates in literature. Yet, for the same systems studied, another well known method, which derives the material parameters from moments of the lateral stress profile, produces results that are neither in accordance with the patch-closure method nor, in fact, physically plausible. One potential reason of the failure lies in the mean field essence of this second method, which does not consider lipid-lipid correlations. Our study hence raises concerns about attempts to derive curvature-elastic properties using the stress profile method.

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Elasticity of Lipid Bilayer Membranes at the Nanoscale: The Need for New Terms

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Transmembrane proteins that have a hydrophobic mismatch with the membrane induce membrane thickness deformations at the nanoscale [1].
We put forward a modification to continuum elastic models describing membrane thickness deformations [2]. We show that contributions involving the gradient (and the Laplacian) of the area per lipid are significant and should be accounted for in the effective Hamiltonian per lipid from which the effective Hamiltonian of the bilayer is constructed, in the spirit of Ref. [3].
We compare the predictions of our model with numerical data giving the profile of membrane thickness close to a mismatched protein [4,5], and with experimental data on gramicidin lifetime [6] and formation rate [7].
This analysis yields consistent results for the term stemming from the gradient of the area per molecule [2]. The order of magnitude we find for the associated amplitude, namely 13-60 mN/m, is consistent with the idea that this term involves a significant contribution of the interfacial tension between water and the hydrophobic part of the membrane. Indeed, this contribution alone would yield a 25 mN/m value for this amplitude. In addition, the presence of this new term explains a systematic variation in numerical data [2].

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Mesoscale Simulations of Curvature Inducing Proteins on Wavy Membranes

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Curvature inducing cell membrane proteins migrate along mean curvature gradients during cell membrane remodeling processes such as endocytosis and cell motility. The curvature sensing abilities of these membrane proteins are vital for their localization and subsequent recruitment of other cell constituents to the membrane. Recent experiments have demonstrated the redistribution of curvature inducing proteins along a precurved membrane supported by a wavy substrate. These experiments can elucidate the behavior of curvature inducing proteins over a much smaller curvature range than was analyzed in previous experiments of segregation on pulled membrane tethers. Wavy substrates provide a model system for deconvolution of the slight effects of frame tension and pinning. The surface migration of these proteins along a wavy surface has been investigated using a curvilinear membrane model evolved with Monte Carlo techniques based on the Helfrich Hamiltonian. The migration and segregation of membrane proteins is quantified in simulations with free energy methods incorporating Widom ghost particle insertion and thermodynamic integration.

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Determining the Mean Curvature Modulus of a Lipid Membrane by Simulating Buckling

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Membrane remodeling is central to a large number of cell biological processes, and the cost for elastically deforming the lipid bilayer features prominently in the energetic budget of such events. It is quantified by the mean curvature modulus, the determination of which is hence a prominent task for experimental and computational membrane scientists alike. The standard approach in simulations is to monitor the undulation spectrum [1], but in order to reach the continuum regime one needs large membranes that take disproportionately long to equilibrate. It has been suggested to instead simulate curved membrane tethers and measure their axial force [2], but this method has technical difficulties for models that are not strongly coarse grained. Here we consider an alternative strategy recently proposed by Noguchi [3], namely, measuring the response of a membrane to buckling. We provide highly accurate analytical expressions to analyze parallel and perpendicular stresses, valid far into the highly nonlinear regime, and we derive fluctuation corrections. Using a variety of membrane models, ranging from strongly coarse grained to atomistic, we show that highly accurate values of the mean curvature modulus can be obtained with remarkable computational ease. The technique also permits to check whether deviations from quadratic curvature elasticity are important, and it offers insights into the thermodynamics of the bending energetics itself.

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Opening Barrier Renormalization by Membrane Local Curvature Fluctuations around the Mechanosensitive Channel: Analytical Expression

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We calculate renormalization of the opening energy barrier of mechanosensitive channel by local curvature fluctuations: $U= U_0 + U_{fl}$, Eq. (1), $P_0(z)$ and $P_1(z,H)$ are lateral pressure profiles in the flat and curved bilayer respectively, H and $A(z)$ are local mean curvature and the difference between open/closed channel cross-section profiles. Function $P_1(z,H)$ was derived in [1] analytically using flexible strings model of lipid chains [2]. The average over fluctuations of the membrane's shape h(x,y) in the Monge representation [3] uses Boltzmann factor of a curved conformation exp(-F(H)/T) with elastic free energy functional F(H) taken in the Helfrich form, Eq. (3); k and r are bending rigidity and surface tension. Comparing our results with molecular dynamics data [4] for curved bilayers, we estimate relative importance of the contributions of the lipid tails and phospholipid headgroups to the energy barrier U.

$$U_0 = \int P_0(z)\Delta A(z)dz\,;\; U_{fl} = \left\langle \int P_1(z,H)A(z)dz \right\rangle_{fl} \quad (1)$$

$$H = div\left[\boldsymbol{\phi}\left(1+\phi^2\right)^{-1/2}\right];\; \boldsymbol{\phi} = \nabla h(x,y) \quad (2)$$

$$F = \int dS\left(\frac{1}{2}kH^2 + r\right) \quad (3)$$

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Membrane Interaction and Curvature Generation by the COPI GTPase Arf1p

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The formation of COPI-transport vesicles and fission from the Golgi membrane proceeds via local deformation of the lipid bilayer by a curvature generating