26th September, 2013

Measuring elastic lipid membrane properties in computer simulations

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Abstract: One of the fascinating aspects of fluid lipid membranes is that on length scales not much bigger than their thickness they can be described exceedingly well by a completely geometric Hamiltonian. Such a continuum-level theory features two main input parameters, namely the moduli describing curvature elasticity. These are called "(mean) bending modulus" and "Gaussian curvature modulus", and their values are not predicted by the effective macroscopic theory. Instead, one either measures them in experiment, or one conducts computer simulations of realistic or coarse-grained membranes which aim at extracting these values. In this talk I will present novel ways for doing the latter. I show that actively buckling a membrane leads to a clean and accurate signal for the mean bending modulus (while making use of the very beautiful and ancient theory of Euler elastica). For the Gaussian modulus one needs to find a way to beat the insidious Gauss-Bonnet theorem, but a protocol that monitors the closure of open vesicle patches permits exactly that. I will also show how our results sometimes fit into existing knowledge and guesses, and how they sometimes trigger perplexing questions for which we do not know the answer yet.

Biography: Markus Deserno is Associate Professor of Physics at Carnegie Mellon University. He studied physics at the Universities Erlangen/Nürnberg and York. In his PhD work at the Max Planck Institute for Polymer Research he investigated counterion condensation for rigid linear polyelectrolytes using theory and simulation. During a postdoctoral stay at the Department of Chemistry and Biochemistry at UCLA he became interested in the biological physics of lipid membranes and viruses. He returned to the MPI-P where he became head of an Emmy Noether Research Group dedicated to studying the biophysics of mesoscopic membrane processes using both continuum theory and coarse grained simulation. His group at Carnegie Mellon works on continuum theory and multiscale modeling of membranes and proteins, applied to problems of both biophysical and biomedical relevance.