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Differentiation of the particle interaction potential in hybrid elastic models and clustering of BAR domains

Abstract:

Hybrid elastic models are used regularly to describe mechanical particle-membrane interactions on a mesoscopic scale where the lipid membrane is approximated by a thin surface and where non-membrane particles are rigid finite-sized entities inducing local deformations along an interface on the membrane surface. In this context the particle interaction potential corresponds to the optimal membrane bending energy at zero temperature subject to a fixed particle configuration. Minimization of this potential is of special interest for various applications, such as for example the investigation of stable particle aggregations.

In this talk we consider a range of hybrid models for which we address existence and numerical accessibility of the gradient of the interaction potential. An existence result may be shown based on an application of the implicit function theorem while numerically feasible representations are obtained from techniques of shape calculus. As a consequence, it is in particular possible to apply gradient-type optimization methods to the interaction potential, which for example enables efficient exploration of stationary particle configurations.