11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20 - 25, 2014, Barcelona, Spain

NUMERICAL AND ANALYTIC COMPUTATION OF ELASTIC INTERACTIONS BETWEEN MEMBRANE PROTEINS

Osman Kahraman[1], Peter D. Koch[2], William S. Klug[3] and Christoph A. Haselwandter[1]

[1] Department of Physics and Astronomy, University of Southern California
[2] Department of Systems Biology, Harvard Medical School
[3] Department of Mechanical and Aerospace Engineering, University of California at Los Angeles

Key Words: *Membrane Mechanics, Membrane Proteins, Computing Methods.*

The elastic theory of membranes provides a successful description of large-scale features of cell membrane mechanics in terms of curvature and area deformations. In the context of interactions between lipid bilayer and membrane proteins, the elastic approach can be extended to include microscopic effects, an important instance being the hydrophobic thickness mismatch at the bilayer-protein interface. For many membrane proteins, such as gramicidin and mechanosensitive ion channels, hydrophobic mismatch yields elastic deformations of the lipid bilayer, inducing long-range interactions between proteins and large-scale organization of membrane proteins into clusters. The elastic energy of protein-induced thickness deformations arises from both stretching/compression of the lipid bilayer and curvature of the two bilayer leaflets, resulting in fourth-order, generalized biharmonic equilibrium equations. Assuming a cylindrically symmetric protein shape and simple far-field boundary conditions, the solution to these differential equations can be expressed analytically as a combination of modified Bessel functions. Using a perturbative approach, we have obtained analytic solutions describing the deformations induced by more than one membrane protein and by proteins having non-axisymmetric shapes. To construct a more general framework for solving the problem of membrane-mediated protein interactions, and to assess the accuracy of analytic methods, we employ both finite-difference and finite-element numerical approximation schemes. We provide error estimates and compare the convergence properties of various implementations of these numerical schemes. We find that a finite-element framework based on mixed interpolation (a discrete Kirchhoff formulation for curvature energy, and a Lagrange interpolation for thickness stretch) is accurate and efficient enough to allow the study of the energetics of infinite and large, finite clusters of membrane proteins. Surprisingly, we find that elastic interactions in clusters of membrane proteins are extremely well approximated by superposition of two-body interactions between neighboring proteins. We make use of this result, along with analytical techniques, to construct fast Brownian dynamics simulations of the formation of membrane-protein clusters.