

PHASE-FIELD MODELING OF VESICLE DYNAMICS: ADHESION AND CONFINEMENT EFFECTS

Christian Peco^{1*}, Daniel Millán² and Marino Arroyo³

^{1,2,3} Laboratory of computational methods and Numerical Analysis (LACÀN)
Universitat Politècnica de Catalunya
Campus Nord UPC, 08034 Barcelona, Spain
e-mail: christian.peco@upc.edu, web page: <http://www.lacan.upc.edu>

Key Words: *Biomembranes, Morphogenesis, Phase-field, Maximum entropy approximants*

Biomembranes are the basic separation structure in cells. Their complex behaviour, rich physical properties and dynamics have been the object of experimental and theoretical investigation for biologists, chemists and physicists for many years. Bio-membranes are made out of several kinds of lipids self-assembled in a fluid bilayer, which presents a fluid behaviour in-plane and solid out-of-plane (curvature elasticity). Vesicles are closed fluid membranes, which play an important role in biophysical processes such as the transfer of proteins, antibodies or drug delivery into the cells. Vesicles serve as simplified models of more complex cell membranes, as well as the basis for bio-mimetic engineered systems. Biomembranes only exist in solution and intimately interact with the surrounding fluid, which owing to the characteristic sizes and velocities, can be modeled with the incompressible Stokes equations.

Phase-field models provide a simple and powerful way to handle multiple effects due to their versatile structure. These models are particularly suitable to be applied on variational schemes where energies can be directly described by the phase-field, thus naturally blending the physics with the diffuse interface. In this paper we start from our previous work on vesicle simulation [1,2] and extend our Lagrangian meshfree [3] phase-field method for biomembrane-fluid flow mechanics from axisymmetry to 3D, exploiting the scientific parallel library PETSc. This model and computer implementation allows us to analyze the dynamics of vesicles under genuinely 3D conditions. In particular, we analyze the morphogenesis of tubular structures under adhesion and confinement [4].

REFERENCES

[1] A. Rosolen, C. Peco and M. Arroyo, An adaptive meshfree method for phase-field models of biomembranes. Part I: approximation with maximum-entropy approximants, *Journal of Computational Physics* (2013), 249:303--319.

[2] C. Peco, A. Rosolen and M. Arroyo, An adaptive meshfree method for phase-field models of biomembranes. Part II: a Lagrangian approach for membranes in viscous fluids, *Journal of Computational Physics* (2013), 249:320--336.

[3]M. Arroyo and M. Ortiz, Local maximum-entropy approximation schemes: a seamless bridge between finite elements and meshfree methods, *International Journal for Numerical Methods in Engineering* 65 (2006), no. 13, 2167-2202.

[4]M.Staykova, M. Arroyo, M. Rahimi and H.A. Stone, Confined bilayers passively regulate shape and stress, *Physical Review Letters* (2013), 110, 028101.