6th European Conference on Computational Mechanics (ECCM 6)
7th European Conference on Computational Fluid Dynamics (ECFD 7)
11 – 15 June 2018, Glasgow, UK

ON THE COMPUTATIONAL MODELING OF CELLULAR MEMBRANES USING ISOGEOMETRIC SHELL ELEMENTS

Roger A. Sauer[1], Amaresh Sahu[2], Yannick A.D. Omar[1] and Kranthi K. Mandadapu[2]

[1] Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University, Templergraben 55, 52056 Aachen, Germany, sauer@aices.rwth-aachen.de, omar@aices.rwth-aachen.de

[2] Department of Chemical & Biomolecular Engineering, University of California at Berkeley, Berkeley, CA, 94720, USA, amaresh.sahu@berkeley.edu, kranthi@berkeley.edu

Key Words: *Helfrich energy, Isogeometric analysis, Non-linear shell theory, Surface flows.*

This work discusses the computational modeling of lipid bilayer membranes based on the nonlinear theory of thin shells [1]. Several computational challenges are identified and various theoretical and computational ingredients are proposed in order to counter them [2]. In particular, C1-continous, NURBS-based, LBB-conforming surface finite element discretizations are discussed [3]. The constitutive behavior of the bilayer is based on in-plane viscosity and (near) area-incompressibility combined with the Helfrich bending model. For quasi-static computations those are complemented by various shear stabilization techniques. For dynamic computations the implicit Euler scheme is used for the temporal discretization. Further, an arbitrary Lagrangian-Eulerian surface formulation is used to handle general surface flows. All ingredients are formulated in the curvilinear coordinate system characterizing general surface parametrizations. Those allow for an extension of the formulation to thermal and chemical coupling [4]. The consistent linearization of the formulation is presented, and several numerical examples are shown.

REFERENCES

[1] R.A. Sauer and T.X. Duong, On the theoretical foundations of thin solid and liquid shells, *Math. Mech. Solids*, Vol. **22**, pp. 343–371, 2017

[2] R.A. Sauer, On the computational modeling of lipid bilayers using thin-shell theory, in D. Steigmann (Ed.), *The role of mechanics in the study of lipid bilayers*, Springer, 2018

[3] R.A. Sauer, T.X. Duong, K.K. Mandadapu and D.J. Steigmann, A stabilized finite element formulation for liquid shells and its application to lipid bilayers, *J. Comput. Phys.*, Vol. **330**, pp. 436–466, 2017.

[4] A. Sahu, R.A. Sauer and K.K. Mandadapu, The irreversible thermodynamics of curved lipid membranes, *Phys. Rev. E*, **96**, 042409, 2017.