

# A finite element method for discoidal lipoprotein particles

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## ABSTRACT

Lipids are the most fundamental constituent of biological structures such as high-density lipoprotein (HDL) particles. These particles consists of a lipid bilayer surrounded by an apolipoprotein belt (apoA-I). The spontaneous shape taken by these particles is not completely understood from first principles, since its size exceeds the capabilities of molecular dynamics computations (unless they are very coarsely grained). Recently, Maleki & Fried discussed the shape stability of a disk endowed with Canham-Helfrich bending stiffness and surrounded by a circular elastic beam as a continuous model of the HDL particle. Their analytic linear-stability analysis only considers infinitesimal perturbations of the planar circular shape. In this communication we will present a fully discrete numerical approximation of the continuous mathematical model and apply it to the investigation of shape evolutions in the fully nonlinear regime. The method uses conforming  $P_1$  interpolants for all fields and discrete differential geometry operators for the computation of mean and Gaussian curvatures of the surface and of the total curvature of the surrounding curve. The time update scheme is fully implicit and based on inexact Newton iterations, with a finite-difference approximation of the Jacobian matrix. The results show that the method is capable of reproducing plane-saddle instabilities arising from the linear analysis, and of computing severely-distorted equilibrium shapes in a robust and convergent manner.