

Supplemental information for TriMem: A Parallelized Hybrid Monte Carlo Software for Efficient Simulations of Lipid Membranes

Marc Siggel,^{*,†,‡,¶,⊥} Sebastian Kehl,^{§,¶} Klaus Reuter,[§] Jürgen Köfinger,[†] and
Gerhard Hummer^{*,†}

[†]*Department of Theoretical Biophysics, Max Planck Institute of Biophysics,
Max-von-Laue-Straße 3, 60438 Frankfurt am Main, Germany*

[‡]*Centre for Structural Systems Biology (CSSB), Notkestraße 85, 22607 Hamburg, Germany*

[¶]*MS and SK contributed equally.*

[§]*Max Planck Computing and Data Facility, Gießenbachstraße 2, 85748 Garching, Germany*

^{||}*Institute of Biophysics, Goethe University Frankfurt, 60438 Frankfurt am Main, Germany*

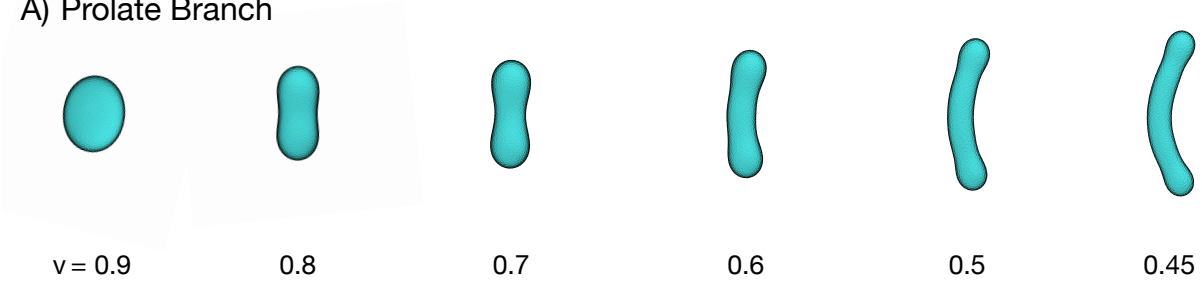
[⊥]*European Molecular Biology Laboratory Hamburg, Notkestraße 85, 22607 Hamburg,
Germany*

E-mail: marc.siggel@embl-hamburg.de; gerhard.hummer@biophys.mpg.de

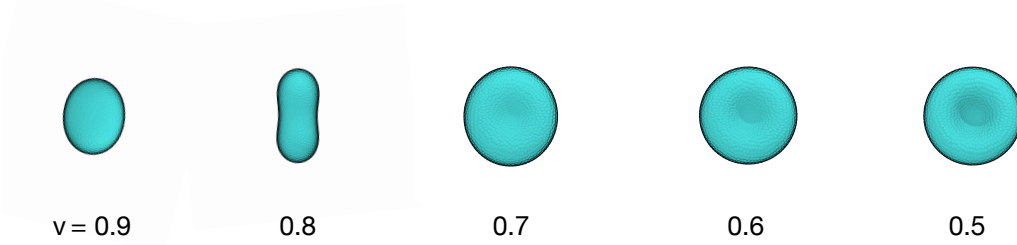
This document contains

- Supplementary Figures
-

A) Prolate Branch



B) Oblate Branch



C) Stomatocyte

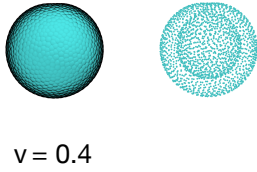


Figure S1: Minimized shapes with $N_V = 1962$ for the phase diagram of varying reduced volume $v = \{0.9, 0.8, 0.7, 0.6, 0.5, 0.45\}$, corresponding to Fig 6. (A) Shapes resulting from simulations initiated on the prolate branch. (B) Shapes resulting from simulations initiated from spheres/prolates. Note that for reduced volumes $v \geq 0.8$, oblate shapes spontaneously transitioned to prolate shapes. (C) Shape of an exemplary stomatocyte at volume $v = 0.4$. For better visibility the same structure is shown with smaller spheres on the right to reveal the inner shape. We note that the neck connecting the two spheres is very narrow. Vertices are shown as large cyan spheres.

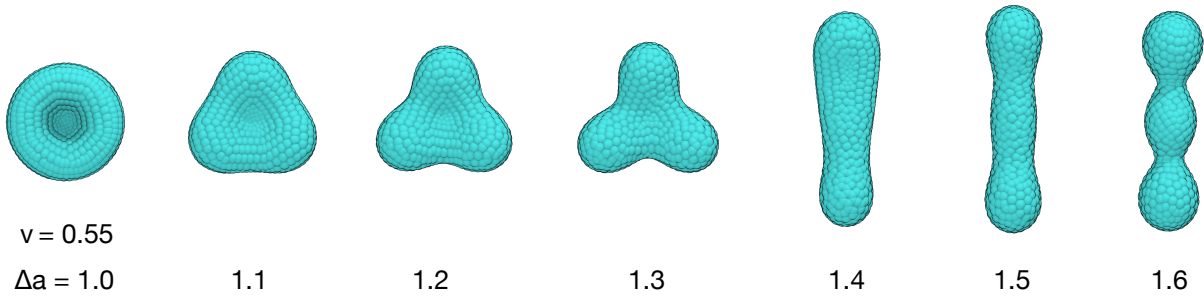


Figure S2: Minimized shapes with $N_V = 642$ for the phase diagram of varying area difference at reduced volume $v = 0.55$, varying area difference ΔA_0 corresponding to Fig 7. Vertices are shown as large cyan spheres.