

# Supporting Material for: “Membrane mediated interactions between circular particles in the strongly curved regime”

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Surface Evolver [K. Brakke, Exp. Math. **1**, 141 (1992)] is a numerical surface optimization program that represents a surface as a simplicial complex (triangulated network) and minimizes its energy (as specified by a surface Hamiltonian) subject to constraints. By using the Helfrich Hamiltonian and implementing bound particles as constraints, we can calculate the force-distance relation between them. In these notes we outline the procedure used by us to perform this task in an automated way.

## 1 Geometric Setup

The initial condition for our Surface Evolver calculations consists of a flat half circle of membrane, embedded in the  $x$ - $y$ -plane, with a radius of  $10,000a$ , where  $a$  is our unit of length (see Figs. 1 and 2 in main article). The flat edge of the membrane is subsequently constrained to lie on the  $x$ - $z$ -plane and along the  $x$ -direction. The semi-circular rim of the membrane patch lies on a half cylindrical constraint. We pick the center of the circle as the origin of our coordinate system. All boundaries are *reflective*, that is, the membrane intersects the boundary constraint surface perpendicularly. Notice that this does *not* fully constrain the membrane’s normal vector on the boundary.

The particle is modeled by two more constraints. It is defined by the radius of the contact line circle between the particle and membrane (we set this to  $a$ , equal to our unit of length) and the contact angle of the membrane at this circle. The particle itself is a spherical cap with radius and center chosen to satisfy these specifications. Vertices inside this spherical cap are constrained to lie on the sphere, and vertices on the contact line are constrained to remain on the contact line.

The particle is initially positioned in the membrane near the flat edge. Since the flat edge is a reflective boundary we can in this manner measure the curvature-mediated force between the particle and its mirror-symmetric image.

## 2 Convergence

Given these constraints Surface Evolver finds the membrane shape that minimizes the bending energy. Here we describe the techniques used to automate the process of convergence. The native Surface Evolver commands used were

<code>hessian_seek</code>	energy minimization step
<code>u</code>	equitriangulation of edges
<code>refine edge</code>	refines a specified edge
<code>delete edge</code>	removes a specified edge

To reduce finite size effects we use a very large patch of membrane (radius  $10,000a$ ), but most of the significant deformation occurs in a small region around the origin. Hence, it is desirable to have a variable level of refinement for the triangulation. We approach this in two ways: First we let the level of refinement depend only on the distance from the center of the particle. After we find a good approximation of the shape, we tune the level of refinement locally based on the curvature of the membrane so that the dihedral angle between facets remains below a maximum value,  $\psi_{\max}$ . The details are as follows:

Initially we assign each edge a length goal,  $l_{\text{goal}}$ , which depends on the distance of the midpoint of the edge from the center of the particle,  $r_{\text{mp}}$ :

$$l_{\text{goal}} = \begin{cases} l_{\text{small}} & \text{if } r_{\text{mp}} < r_{\text{small}} \\ \frac{r_{\text{mp}}}{r_{\text{small}}} l_{\text{small}} & \text{if } r_{\text{mp}} > r_{\text{small}} \end{cases}, \quad (1)$$

where  $r_{\text{small}} = 4a$  is a distance that is large enough such that the particle is initially in this area of higher resolution, and  $l_{\text{small}}$  is the desired edge length within this area of high resolution. We start with  $l_{\text{small}} = a$ .

We then converge towards the minimum energy. This involves several steps. We call `hessian_seek`, refine all edges that have a length greater than  $3l_{\text{goal}}$ , equitriangulate the edges, delete all edges with lengths smaller than  $l_{\text{goal}}$ , and equitriangulate again. This process is repeated until the energy converges to a constant value. Typically, we use a relative error tolerance of  $10^{-8}$  of the total energy.

After convergence we reduce  $l_{\text{small}}$  by a factor of two and repeat the procedure. This refinement process is then repeated once more, after which we reach a reasonable starting resolution of  $l_{\text{goal}} = a/4$ . We now have arrived at an approximation of the membrane shape and base further refinement not just on

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the distance of any local vertex from the center of the particle, but also on the local *curvature* of the membrane. An integer representing the refinement level is associated with each *facet*. Initially all facets have a refinement level of 0. A maximum dihedral angle is specified,  $\psi_{\max}$ , which should not be exceeded by any dihedral angles between facets. All facets which have a dihedral angle with any of their neighbors that is larger than  $\psi_{\max}/2$  are found and their refinement levels are increased by 1. Then, with a 20% probability, the refinement level of all facets whose dihedral angles are smaller than  $\psi_{\max}/6$  are increased by 1. Finally, each facet's refinement level is updated by averaging its own level with that of its neighbors (its own is given a weight of 1/2 and the neighbors 1/6). This averaging improves stability.

We now define the refinement level,  $\lambda$ , of an *edge* to be the average of the refinement levels of its two neighboring facets, and from this the new value for  $l_{\text{goal}}$  is calculated:

$$l_{\text{goal}} = 1.5^{-\lambda} \times \begin{cases} l_{\text{small}} & \text{if } r_{\text{mp}} < r_{\text{small}} \\ \frac{r_{\text{mp}}}{r_{\text{small}}} l_{\text{small}} & \text{if } r_{\text{mp}} > r_{\text{small}} \end{cases} \quad (2)$$

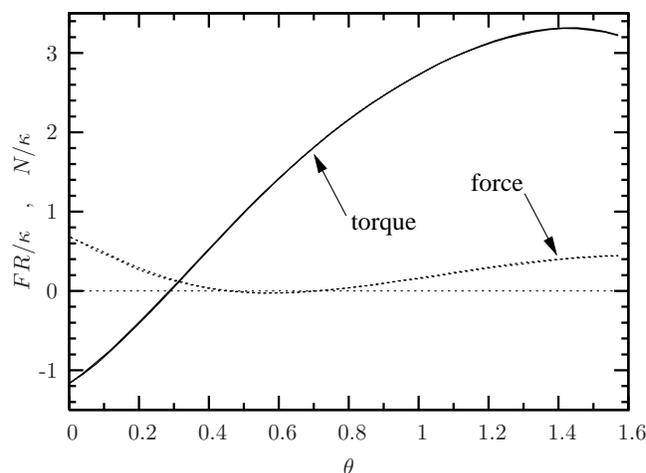
The process of minimizing, refining, equilibrating, and deleting is repeated until convergence is reached. If there remain any dihedral angles larger than  $\psi_{\max}$  we adjust the refinement levels of the facets again, converge again, and repeat until no dihedral angles exceeds the specified maximum.

### 3 Measurement of Forces and Torques

To determine the force and torque that a particle is experiencing, we measure the energy change of an incremental change in its position or orientation, respectively. A typical change is  $10^{-10}$ . One can think of this as measuring the response to a “virtual displacement”, which directly probes the corresponding constraint forces and torques. Importantly, no convergence of the membrane shape is performed after the shift in position or orientation before measurement of the energy. The latter point is very essential: It permits us to compare energies which are based on the *same* triangulation. This eliminates the numerical noise associated with different triangulations.

### 4 Movement and Tilting of the Particles

Performing the small shifts for forces and torque measurements is trivial, but making larger shifts necessary to change the position and orientation of the particles in the membrane is more difficult. This is because translating or tilting the particle more than just infinitesimally requires moving the surrounding membrane with it. When the particle is translated a distance  $d$ , the distances  $r_{\text{vert}}$  of all membrane vertices from the particle are calculated (this is the distance from the vertex



**Fig. 1** Force  $F$  and torque  $N$  acting upon a particle as a function of particle tilt  $\theta$ . The particle-particle distance is  $r = 2.8a$  and the particle/membrane contact angle is  $\alpha = \frac{\pi}{4}$ .

to the closest point on the circle bounded by the particle contact line). Then the distance from the particle to the nearest other constraint (*i.e.* to the edge of the membrane patch)  $r_{\max}$  is also found and each vertex is translated a distance  $d_{\text{vert}}$ , in the same direction as the particle, given by

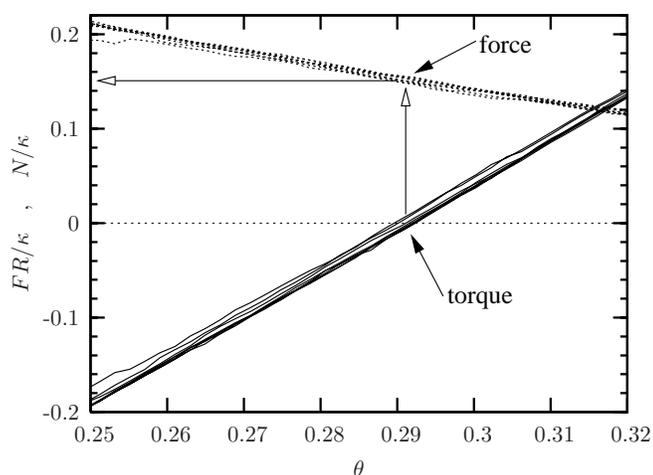
$$d_{\text{vert}} = \begin{cases} \frac{d}{2} \left[ \cos\left(\frac{\pi r_{\text{vert}}}{r_{\max}}\right) + 1 \right] & \text{if } r_{\text{vert}} < r_{\max} \\ 0 & \text{if } r_{\text{vert}} > r_{\max} \end{cases} \quad (3)$$

In this manner the surrounding membrane is moved with the particle without introducing any kinks that would introduce numerical instability. The rotation of the particle is performed in the same manner, except that the surrounding membrane is rotated with rather than translated with the particle and it is the angle of rotation rather than the displacement that is modified.

Of course, this procedure only creates a convenient and partially pre-equilibrated *initial configuration*, which subsequently needs to be energy minimized as described in the previous section.

### 5 Calculation of a Force-Distance curve

To illustrate the calculation of a curvature-mediated force, let us pick the example of two particles with a contact angle of  $\alpha = \frac{1}{4}\pi$  and a separation of  $2.8a$ . For the maximum allowed dihedral angle we tried both  $\psi_{\max} = 0.05$  as well as  $\psi_{\max} = 0.05\alpha$  (for small  $\alpha$ ), but the final results did not strongly deviate. The system is initialized with the particle oriented horizontally ( $\theta = 0$ ) at a distance of  $2.0a$  from the planar boundary condition (corresponding to a particle-particle separation of  $r = 4.0a$ ). The particle is slowly rotated until it

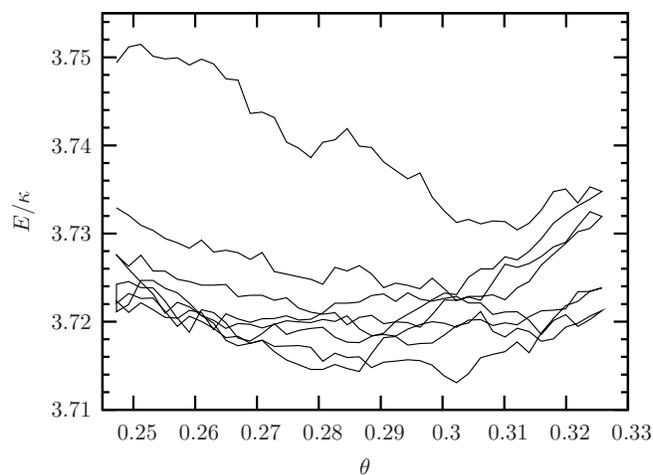


**Fig. 2** Force  $F$  and torque  $N$  acting upon a particle as a function of particle tilt  $\theta$ . The particle-particle distance is  $2.8a$  and the particle/membrane contact angle is  $\frac{\pi}{4}$ . Four scans back and forth of the particle tilt are shown. The force corresponding to the zero-torque-condition is the one which is physically realized.

is vertical, parallel to the planar boundary condition ( $\theta = \frac{\pi}{2}$ ). This rotation is performed in small steps, and after each step the surface is relaxed to its minimum energy shape. The particle is then gradually moved toward the planar boundary condition until the desired distance of  $1.4a$  is achieved, again minimizing the surface energy after each small step. This procedure (starting at a somewhat larger distance and then gradually inching closer) might seem overly complicated; however, this “detour” is necessary if the final distance is closer than  $1.0a$ , and for consistency reasons we used the same protocol also for larger distances.

From this initial state the particle is tilted in small steps from  $\theta = \frac{\pi}{2}$  to  $\theta = 0$ . After each small step the force and torque acting on the particle is measured. The process is then reversed and the particle is gradually tilted until it is again vertical. The force- and torque-traces for this process are shown in Fig. 1. Notice that the results for both scan directions essentially overlap, indicating that under these conditions the process is reversible (*i.e.*, it doesn’t show “numerical hysteresis”). We now identify the tilt angle at which the torque vanishes, since this corresponds to the equilibrium configuration which a particle (at this separation to its mirror-symmetric partner and this value for the curvature imprint  $\alpha$ ) will assume if it is orientationally unconstrained. To determine the curvature-mediated force that such particles would experience, we would simply have to find the value of the force corresponding to this zero torque condition. However, the large step size used in these traces renders the corresponding result too inaccurate. A further refinement is needed.

The tilt-scans are thus repeated, but rather than scanning



**Fig. 3** Membrane bending energy  $E$  as a function of particle tilt  $\theta$ . The particle-particle distance is  $2.8a$  and the particle/membrane contact angle is  $\frac{\pi}{4}$ . Four scans back and forth of the particle tilt are shown.

back and forth over the entire range of orientations from vertical to horizontal, the orientation is scanned back and forth only over a relatively narrow region over which the torque is now known to pass through zero. Typically we scan back and forth four times. The results of such a scan are shown in Fig. 2. Although each repeat overlaps approximately with the previous ones, discrepancies can be clearly seen. The reason for this is that the triangulation used to model the membrane is constantly changing, and this effects the measured forces and torques slightly. We calculate the force at zero torque for each pass by fitting a line to the 6 points nearest to the intercept, and use the scatter of the calculated forces as an indicator for the error due to the finite triangulation size of our model.

The reader may also have noticed that so far we have not yet presented any of the measured *energies*. As explained previously, the error introduced by the changing triangulation makes comparison of calculated energies difficult. This can be clearly seen in Fig. 3, where we plot the measured energy during the above scans. This error in the calculated energy would seem problematic since we measure our forces and torques by making small changes to the position and orientation of the particle and looking at the change in energy. The forces and torques obtained from “virtual displacements” always compare energies based on the *same* triangulation, thereby eliminating much of the triangulation noise. As the reproducibility of the force and torque data in Fig. 2 proves, this method is trustworthy.