Supplementary Information for "Dynamics of self-assembly of model viral capsids in the presence of a fluctuating membrane"

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We define the various functions used in the interactions between particles and in the confinement of the membrane particles to the frame. The repulsive, U_{rep}, and attractive, U_{att}, radial potentials used for inter-sub-unit and sub-unit-membrane interactions are given by,

$$U_{rep}(r) = \begin{cases} 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} + \frac{1}{4}\right] & \\ & \text{for } r < r_t, \\ 0 & \\ & \text{for } r \geq r_t, \end{cases} \tag{1}$$

and

$$U_{att}(r) = \begin{cases} -\epsilon & \\ & \text{for } r < r_t, \\ 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] & \\ & \text{for } r_t \leq r \leq r_s, \\ a(r-r_c)^2 + b(r-r_c)^3 & \\ & \text{for } r_s \leq r \leq r_c, \\ 0 & \\ & \text{for } r \geq r_c, \end{cases} \tag{2}$$

where r is the particle center separation, $r_t = 2^{1/6}\sigma$, $r_s = (\frac{26}{7})^{1/6}\sigma$, $r_c = \frac{67}{48}r_s$, $a = -\frac{24192}{3211}\frac{\epsilon}{r_s^2}$ and $b = -\frac{387072}{61009}\frac{\epsilon}{r_s^3}$. In the range $r_s \leq r \leq r_c$, a polynomial interpolation is used for $U_{att}(r)$ so that the potential goes smoothly to 0.[1]

Patchy interactions are produced by multiplying U_{att} by $\gamma_{orient}(\hat{\boldsymbol{r}}_{ij}, \Omega_i, \Omega_j)$, where $\hat{\boldsymbol{r}}_{ij}$ is the unit vector pointing between the particle centers and Ω_i an orientation. For inter-sub-unit interactions, γ_{orient} is composed of three, and for membrane-sub-unit interactions only one, factor of the

following functional form,[2]

$$F(\theta;\theta_0,\theta_1) = \begin{cases} 1 & \\ & \text{for } \theta \le \theta_0, \\ \cos^2[(\pi/2)(\theta-\theta_0)/\theta_1] & \\ & \\ & \text{for } \theta_0 \le \theta \le \theta_0+\theta_1, \\ 0 & \\ & \text{for } \theta \ge \theta_0+\theta_1, \end{cases} \tag{3}$$

where θ_0 and θ_1 are parameters that define patch width.

The bond interaction between two bonded membrane particles, i and j, is given by[3]

$$U_{bond}(r_{ij}) = \begin{cases} 0 & \\ & \text{for } r_{ij} \le 1.15 l_0, \\ (80 k_B T)\exp[1/(1.15l_0 - r_{ij})]/(1.33l_0 - r_{ij}) & \\ & \\ & \text{for } 1.15l_0 < r_{ij} < 1.33l_0, \\ \infty & \\ & \text{for } r_{ij} \ge 1.33 l_0, \end{cases} \tag{4}$$

with $r_{ij} = |\mathbf{r}_{ij}| = |\mathbf{r}_j - \mathbf{r}_i|$, where $\mathbf{r}_i$ is position of particle i. Additionally, an excluded volume

potential is applied between all pairs of membrane particles

$$U_{EV}(r_{ij}) = \begin{cases} \infty & \text{for } r_{ij} \leq 0.67 l_0, \\ (80 k_B T) \exp[1/(r_{ij} - 0.85 l_0)]/(r_{ij} - 0.67 l_0) & \text{for } 0.67 l_0 < r_{ij} < 0.85 l_0, \\ 0 & \text{for } r_{ij} \geq 0.85 l_0. \end{cases} \tag{5}$$

These potentials set minimum distance between membrane particles to $0.67 l_0$ and the maximum bond length to $1.33 l_0$. The total area, A, of the membrane is constrained with a potential,

$$U_{area} = (k_B T)(A - A_0)^2, \tag{6}$$

where $A_0 = (\sqrt{3}/4) l_0^2 N_{tri}$ and N_{tri}, the number of triangles in the membrane surface, may vary. Membrane particles forming the edge of the surface are confined to a frame region, located a distance r_{frame} into the simulation box. Within a volume of cross-section $l_0 \times 4 l_0$, where the larger extension is out of the plane in which the membrane would be extended in a stretched configuration, confined membrane particles experience a flat potential of E_{frame}. E_{frame} may be used to control the average of r_{frame} and is set by comparison with tensionless simulations performed with box rescaling.[4] When confined membrane particles move out of the central part of the frame they experience a potential essentially identical to that used for excluded volume,

$$U_{confine}(r) = \begin{cases} E_{frame} + (80 k_B T) \exp[-1/r]/(0.18 l_0 - r) & \text{for } 0 < r < 0.18 l_0, \\ \infty & \text{for } r \geq 0.18 l_0, \end{cases} \tag{7}$$

where r is the distance of the confined membrane particle from the closest point within the flat-potential region.

References

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