Electronic Supplementary Material (ESI) for Soft Matter.

Interplay of particle shape and suspension properties: A study of cube-like particles—Electronic Supplementary Information

Debra J. Audus,*[a] Ahmed M. Hassan,[a] Edward J. Garboczi,[b] and Jack F. Douglas*[a]

1 ZENO: Code modifications

The special cases of the cube ($s \to \infty$) and the sphere ($s = 0$) are already implemented in the ZENO code available online. Thus, for these cases, the code was used as is. However for all other values of s of interest, code modifications were required. Specifically, three functions needed to be written. The first function, maxshape, determines the size of the sphere that circumscribes the cube-like particle. The second function, proshape, determines the smallest cuboid that surrounds the cube-like particle. The final function, minshape, determines the shortest distance between a specified point and the cube-like particle.

The first two functions were straightforward. Taking $a = 1$ and the origin as the center of the cube-particle, the radius of the sphere that circumscribes the cube-like particle is $3^{\frac{1}{2}-\frac{1}{2s}}$, and the cuboid that surrounds the cube-like particle is always a cube centered at the origin with side lengths of 2.

However, determining the shortest distance between a specified point and the cube-like particle requires numerical calculations. Noting that symmetry allows us to only consider the problem in one octant and given a point (x_p, y_p, z_p), the distance squared between that point and a point on the cube-like particle's surface at θ and φ is

$$d^2 = x_p^2 + y_p^2 + z_p^2 + r^2(\theta,\varphi) - 2r(\theta,\varphi)[|x_p||\cos(\varphi)||\sin(\theta)| + |y_p||\sin(\varphi)||\sin(\theta)| + |z_p||\cos(\theta)|] \quad (1)$$

where $r(\theta,\varphi)$ is the radius defined in Eq. 10 in the main text. This function is then minimized with respect to θ and φ using the downhill simplex method.[1] Note that by taking the absolute values of each of the trigonometric functions, the minimization becomes unconstrained. Although the returned values of θ and φ may not be in the first octant, their values can be mapped to the first octant and the value of d^2 is unaffected due to symmetry. The distance is then computed from d^2. For the downhill simplex method, we used a tolerance of 10^{-8}; this value was small enough that the results were independent of its choice given the chosen skin thickness of 10^{-4}.

2 SCUFF-EM: Meshing algorithm

The surface mesh for SCUFF-EM was generated by placing nodes on the surface of object uniformly every $\Delta\theta = \Delta\varphi = \pi/60$ in the range $\pi/60 \le \theta \le 59\pi/60$ and $\pi/60 \le \varphi \le 119\pi/60$. In addition, a node is placed at the top and bottom of the surface of the object which correspond to the points $\theta = 0$ and $\theta = \pi$, respectively. The previous scheme yields a total of 6962 nodes. The nodes are then connected with a triangular mesh as shown in Fig. 1 for $s = 2.5$.

[a] *National Institute of Standards and Technology, Gaithersburg, MD Email: debra.audus@nist.gov, jack.douglas@nist.gov*
[b] *National Institute of Standards and Technology, Boulder, CO*

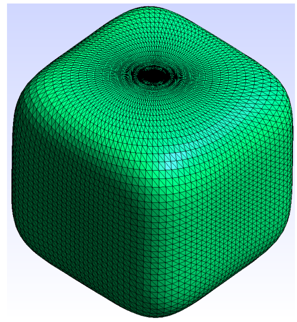

Figure 1 Illustration of the mesh for SCUFF-EM with $s = 2.5$.

3 Computational resource requirements

Since we used three different methods that are realizations of three different algorithms, we compared the required computational reources for $[\sigma]_\infty$ with $s = 1.5$ and $s = 10$. The three algorithms considered where numerical path integration (ZENO), boundary element (SCUFF-EM) and finite element (COMSOL). There results can be found in Table 1. Due to the differences in approach, we increased the resolution for all three methods until the value of $[\sigma]_\infty$ changed by less than 0.1%. For numerical path-integration, boundary element and finite element, this corresponded to ten thousand random walks for $s = 1.5$ and one hundred thousand random walks for $s = 10$, 3,042 nodes, and a maximum finite element size of 0.2, respectively. All runs were performed on a single core Intel® Xeon® CPU E5620 processor[2] with a clock speed of 2.4 GHz and 12 MB cache memory. We found that the computational times were generally comparable and that although the difference in memory requirements was more substantial, it may not be of concern depending on the available computational resources. We emphasize that the computational times and memory requirement were not prohibitive. Thus we did not optimize the mesh in order to reduce the computational burden, which means that our results are approximations of the expected computational requirements.

Table 1 Comparison of CPU and memory requirements for the calculation of $[\sigma]_\infty$ for the three computational methods.

	s	path-integral (ZENO)	boundary element (SCUFF-EM)	finite element (COMSOL)
Run time (min)	1.5	5	12	9
Memory (MB)	1.5	19	326	14100
Run time (min)	10	64	15	56
Memory (MB)	10	19	326	14800

References

[1] J. A. Nelder and R. Mead, *Comp. J.*, 1965, **7**, 308–313.

[2] Certain commercial equipment and/or materials are identified in this report in order to adequately specify the experimental procedure. In no case does such identification imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the equipment and/or materials used are necessarily the best available for the purpose.