Supplementary Materials

Reducing grid-dependence in finite-difference Poisson-Boltzmann calculations

Jun Wang,[1,†] Qin Cai,[1,2,†] Ye Xiang,[1,3] and Ray Luo[1,2]

1. Department of Molecular Biology and Biochemistry
University of California, Irvine, CA 92697, USA
2. Department of Biomedical Engineering
University of California, Irvine, CA 92697, USA
3. Department of Physics,
Shanghai Normal University, Shanghai 200234, China

Geometrical Method to Compute Intersection Points

In WHA or NHA, we need to calculate the intersection point between the grid edge and the molecular surface. In the manuscript, we have described a simple algebraic method to compute the intersection points. Here for the sake of completeness and comparison, we describe a comparable method that is often used in the literature, *i.e.* via geometric relations among different atoms and probe spheres.

Denote the inside and outside grid point as M and N, respectively, and their labels as LM and LN, respectively. Suppose their corresponding owners, *i.e.* atom or probe spheres, are OM and ON with radii RM and RN, respectively. If an owner sphere OM

intersects the grid edge, we denote the intersection point as PM. Similarly we denote the intersection point of an owner sphere ON and the grid edge as PN. The intersection point is assigned based on the following rules, and shown in Figure S-1.

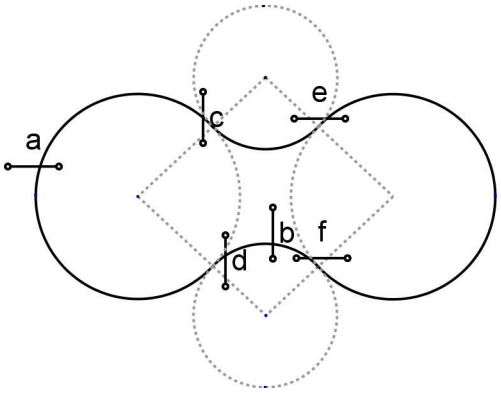

Figure S-1. Various scenarios (a-f) of intersection point assignment. The diagram shows two atoms jointed by the reentry volume. The solid line represents the SES surface. The dotted circles represent solvent probes. The dotted diamond represents the reentry cones formed by the solvent accessible arc and the two atomic centers.

1. If LM=-2 and LN=2, the required intersection point is PM, *i.e.* the intersection point with the van der Waals sphere/contact surface is computed with the atom whose surface is closest to M. (Figure S-1: segment a)
2. If LM=-1 and LN=1, the required intersection point is PN, *i.e.* the intersection point with the reentry surface is computed with the closest solvent probe to N. (Figure S-1: segment b)
3. If LM=-1 and LN=2, and if PN is outside the reentry cones, the required intersection point is PN, otherwise, it is PM. (Figure S-1: segments c and d)
4. If LM=-2 and LN=1, and if PM is outside the reentry cones, the required intersection point is PM, otherwise, it is PN. (Figure S-1: segments e and f)

It should be pointed out that it is not guaranteed that the geometric algorithm outlined above can always calculate the intersection points correctly. However, the error due to the incorrect calculation should, in principle, reduce when the grid spacing

is reduced. Figure S-2 illustrates a simple situation where the algorithm may fail. The intersection plane shown in Figure S-2 goes through the solvent accessible arc of two neighbor atoms. The dash line represents the arc points and the solid line represents the SES surface. Point *j* and *j+1* are two neighbor grid points. Since they are in the reentry region, point *j* is labeled as 1 and point *j+1* is labeled as −1. Their corresponding owners are C+ and C−, respectively. Figure S-2 shows that the correct intersection point of the grid edge and the SES surface is point P, sphere C+ intersects the grid line at P', and sphere C− does not intersect the grid line. Thus the above algorithm returns P' as the intersection point. Apparently the failure is due to the fact that the true intersection point P can never be derived from the knowledge of point *j*, *j+1*, C+, and C− alone. Of course the error certainly becomes smaller when the grid spacing becomes smaller. That is to say the algorithm does have the correct convergence behavior with respect to the grid spacing.

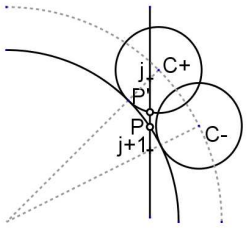

Figure S-2. Limitations of the geometric method for calculation of the intersection points between the molecular surface and grid edges.