Title: A fast method for evaluating Green’s function in irregular domains with application to charge interaction in a nanopore

Author: Qiyuan Zhao

Supervisor: Zhenli Xu

Method: The algorithm is based on two-level image charges, in which the inner-layer charges are located nearby the boundary to eliminate the singularity of the induced polarization potential, and the outer-layer charges with fixed positions approximate the long-range tail of the potential.

Results:

We find the number of inner-layer image charges can be very small and thus the total complexity of the algorithm is less expensive and potentially suitable for use in particle simulations.

Note:
The whole work is accepted by "communications in computational physics".

Fig. Schematic illustration for the solution of the Green’s function.

Fig. (ab) Absolute error of the self-energy for the source charge located at (1,1,1) as function of d: (a) without and (b) with inner-layer images. (cd) Maximum error in the induced potential: (c) without and (d) with inner-layer images.