Robust boundary integral formulation of Debye-Hückel model

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The calculation of electrostatic interactions in liquids is needed in many chemical and biological applications, including electrostatic interactions between colloid particles, emulsions, and electrostatic interactions between charged proteins as well as drug-substrate interactions.

The Debye-Hückel (linearized Poisson-Boltzmann) model is an effective implicit continuum model to study electrostatic interactions. The boundary integral method is a general, flexible and efficient way to solve problems that arise in the Debye-Hückel model [1-3], as it reduces the dimension of the calculation domain by one. However, there are some drawbacks in the traditional boundary integral method because of the singularities of the Green's function and its normal derivative.

In this talk, we will introduce a novel, robust and non-singular boundary integral method in which all the singular behaviors in the integrands have been analytically eliminated. As such, compared to the traditional boundary integral method, our method is able to calculate accurately the interactions between two objects of general shape even when their surfaces are close (see Fig. 1).

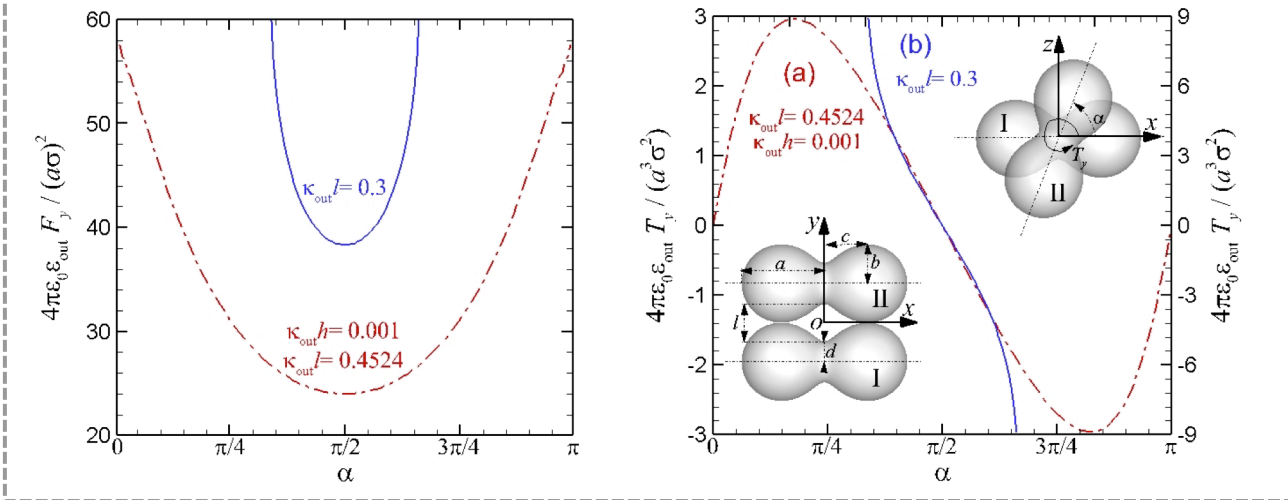

Figure 1 Dimensionless force, F_y, and torque, T_y, due to electrical double layer interactions between two closely spaced dumb-bell shaped particles at constant surface charge, σ, as functions of relative orientation, α, obtained using our non-singular boundary integral method. The dimensionless geometric parameters are: κa = 1, κb = 0.4757 and κd = 0.25, for values of κl shown in the figure.

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