How to implement the short solvent system for biosimulation?

In this note I will breifly describe my preliminary idea on how to implement the short solvent system for biosimulation. In our draft we already described the short solvent system for ion pairs solvated in water. In summary, in the short solvent system the wate-water and ion-water Coloumb interaction are GT truncated. The ion-ion Coloumb interaction is an effective interaction determined by Eq (17) in main 9.pdf.

One problem of the effective ion-ion Coloumb interaction is that it depends on the water charge distribution around the ion, as shown in Eq (17). This means that the effective Coloumb interaction is different between different types of ions. For example, the $Na^+ - Cl^-$ effective interaction will be different from the $K^+ - Cl^-$ or $Ca^{2+} - Cl^-$ effective Coloumb interaction. This will be a big problem for biosimulation, since there are so many different

types of atoms in a protein. For example, the Carbon atom appearing at different locations of the side chain has different LJ parameters and partial charges. If we want to get the effective interaction for all those atom types using Eq(17), we need to calculate the water charge distribution around all these atoms, which is too time consuming to be done.

To solve this problem I propose the following simplification: we just assume the effective Coulomb interaction is universal between any atoms. This means that, for example, the effective interaction between A and B is $q_A q_B v^*(r)$, and the effective interaction between A and C is $q_A q_C v^*(r)$, where $v^*(r)$ is the universal effective Coulomb interaction.

This assumption of the universal effective Coloumb interaction is equivalent to assuming the water charge distribution around an atom is universal after scaled by the atom charge. Since the charge distribution is convoluted with the slowly-varying $v_i(r)$, the small differences in the charge distribution wouldn't really matter, which makes my assumption not too bad.

As an evidence to support this assumption, the

effective Coloumb interaction between $Na^+ - Cl^-$ is not two different from the one between $Ca^{2+} - Cl^-$.

I tried to determine $v^*(r)$ by fitting with the $Na^+ - Cl^-$ and $Ca^{2+} - Cl^-$ effective Colomb interaction.

The $v^*(r)$ determined has the following form

$$v^*(r) = v_0(r) + \frac{0.78}{\epsilon} e^{-0.75\left(\frac{r}{\sigma}\right)^2} + \frac{1}{\epsilon}\frac{\mathrm{erf}\left(\frac{r}{\sqrt{2}\sigma}\right)}{r},$$

where $\epsilon = 71$ is the dielectric constant for SPC/E, and $\sigma = 0.5$ nm is the smoothing length.

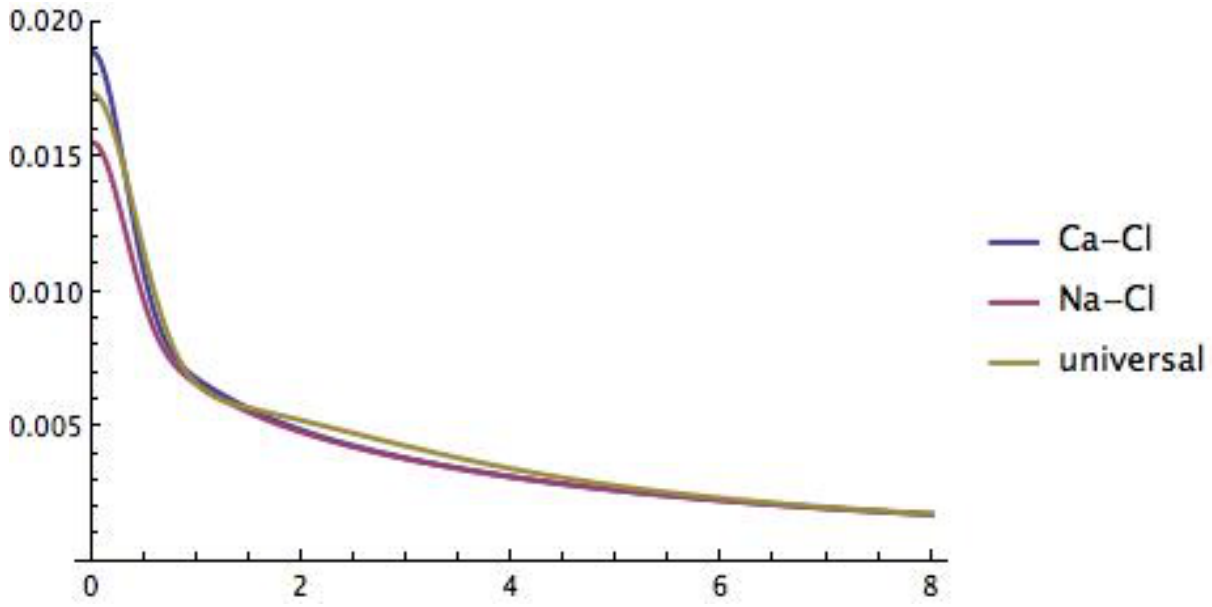
This $v^*(r)$ consists of three parts:

$v_0(r)$ — the short ranged GT interaction.

$\frac{0.78}{\epsilon} e^{-0.75\left(\frac{r}{\sigma}\right)^2}$ — the middle ranged interaction

$\frac{1}{\epsilon}\frac{\mathrm{erf}\left(\frac{r}{\sqrt{2}\sigma}\right)}{r}$ — the long ranged tail.

The first two parts are finite ranged. The last part can be calculated directly using Ewald sum.



The figure above shows how $v^*(r)$ is compared to the effective $Na^+ - Cl^-$ and $Ca^{2+} - Cl^-$ Coloumb interaction. Notice that the $v_0(r)$ is not shown in this plot. As you can see they are not too far away from each other!

In biosimulation I suggest we use $v^*(r)$ for the interaction between atoms on the protein.