

# Supplementary material: Adaptive resolution simulation of salt solutions

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## 1. System with SPC water molecules

The system with SPC [1] water molecules has a box size of 16.20 x 4.05 x 4.05 nm with 8508 water molecules, 160 Na and 160 Cl ions, which corresponds to 1 M NaCl solution. The rest of the simulation setup is as described in the original paper. Following are results for the SPC system, which are similar to the SPC/E [2] system and thus not included in the original paper [3].

## 2. Results for the SPC system

We calculate radial distribution functions (RDF) for atomistic, coarse-grained, and AdResS simulation as for the SPC/E system. Figures 1, 2 and 3 show RDFs (bottom) and effective pair potentials (top) for water-water center of mass, water-Cl and water-Na respectively. For the AdResS simulations two RDFs are shown, one where we average only over molecules in the explicit atomistic (ex) domain and the other where we average only over molecules in the coarse-grained (cg) domain. As in the original paper, one can see that the obtained effective pair potentials produce RDFs that match the reference atomistic RDF.

We calculate the normalized density profile (NDP) along the x-coordinate for centers of mass water molecules and for the ions to verify the density is homogeneous across the different regions of the simulation box. Figure 4 shows the thermodynamic forces used for the corresponding molecule types for the SPC system. The obtained thermodynamic forces are similar to those for the SPC/E system. Figure 5 depicts  $NDPs_{cm}$  for all three molecule types. NDPs are shown along the x-coordinate, as this is the direction in which the resolution of the molecules changes. Shown are NDPs from three simulations: all-atom (bottom), AdResS with thermodynamic forces acting on all molecule types (middle) and AdResS with thermodynamic forces acting on water molecules only (top). As in the SPC/E system, one can clearly see that thermodynamic forces on ions are also needed for a flat density profile.

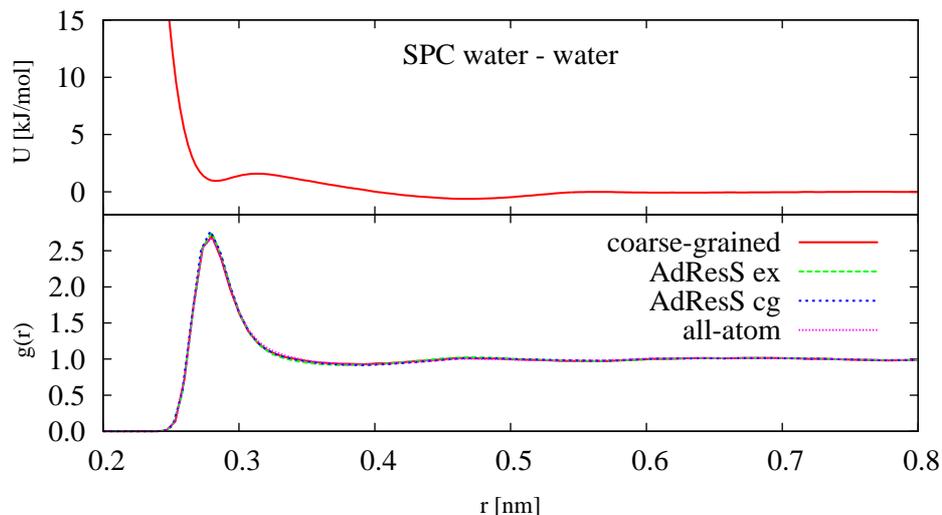


Figure 1: Radial distribution functions of water-water centers of mass for the system with SPC waters (bottom). Effective pair potential for water-water center of mass interactions between molecules (top). Atomistic  $RDF_{cm}$  is well reproduced by the coarse-grained and AdResS simulations (both in the explicit atomistic (AdResS ex) and coarse-grained (AdResS cg) domains).

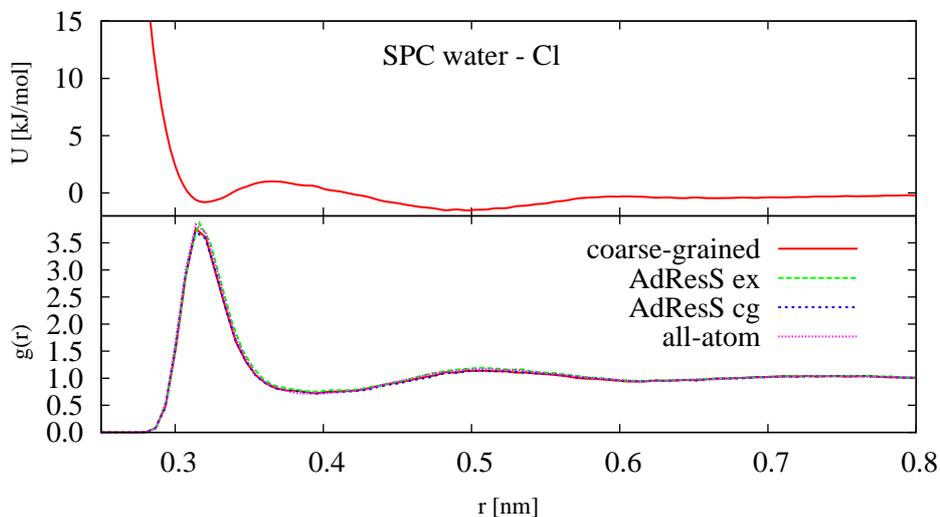


Figure 2: Water-Cl radial distribution functions for the system with SPC waters (bottom). Effective pair potential for water-Cl center of mass interactions between molecules (top). Atomistic  $RDF_{cm}$  is well reproduced by the coarse-grained and AdResS simulations (both in the explicit atomistic (AdResS ex) and coarse-grained (AdResS cg) domains).

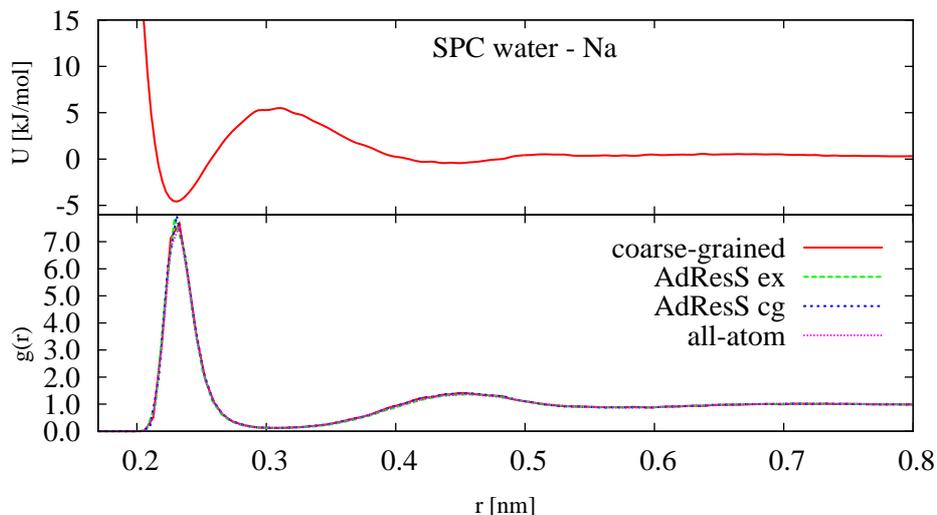


Figure 3: Radial distribution functions of water-Na center of mass molecules for the system with SPC waters (bottom). Effective pair potential for water-Na center of mass interactions between molecules (top). Atomistic  $RDF_{cm}$  is well reproduced by the coarse-grained and AdResS simulations (both in the explicit atomistic (AdResS ex) and coarse-grained (AdResS cg) domains).

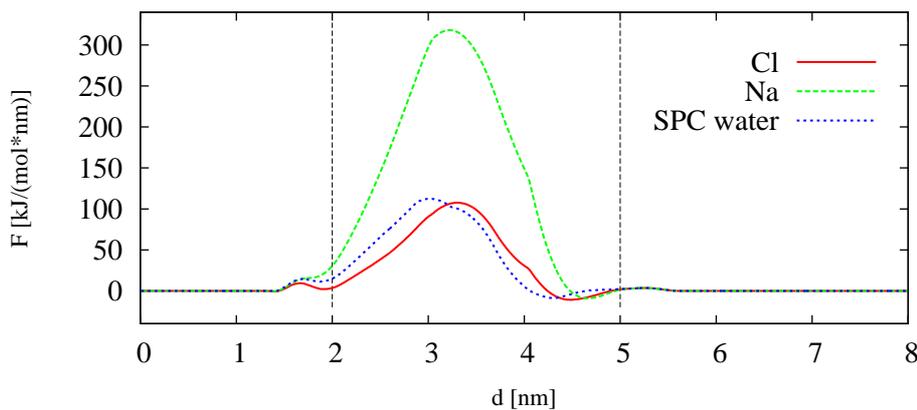


Figure 4: Thermodynamic forces used in the SPC system for the corresponding molecules. The x-axis shows the distance from the center of the simulation box in x-direction. Vertical lines denote the boundaries of the hybrid region. The thermodynamic force is symmetric about  $d = 0$ .

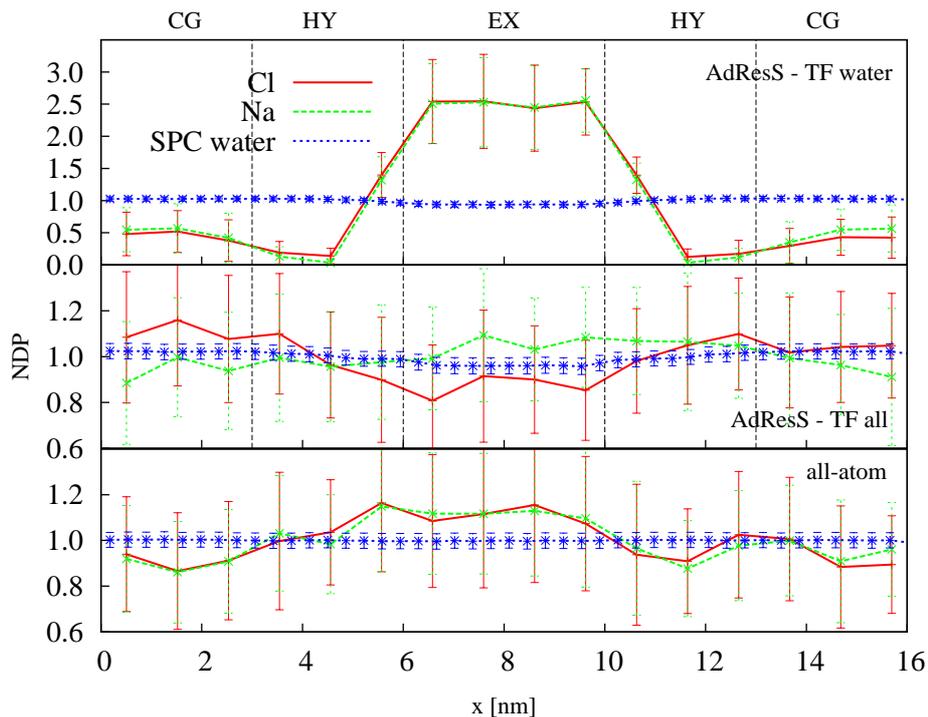


Figure 5: Normalized density profiles along the x-coordinate for the system with SPC waters for water center of mass of molecules and ions. For each species its corresponding bulk density is taken for normalization. Top and middle plots show AdResS simulations where vertical lines mark the boundaries between different resolutions. In the middle plot thermodynamic forces are applied to all three molecule types. At the top are shown normalized density profiles where thermodynamic force is added to water molecules only. This clearly shows that the ions distributions are decoupled from water molecules and that thermodynamic forces on ions are needed for a flat density profile. At the bottom are shown normalized density profiles of an all-atom simulation. Ion density fluctuations of the same order of magnitude as in the AdResS simulation are present. The plots include error bars.

To check the dynamical properties we have monitored mean square displacements (MSD) of different molecular species. Figure 6 shows MSDs for all-atom, AdResS and coarse-grained simulations.

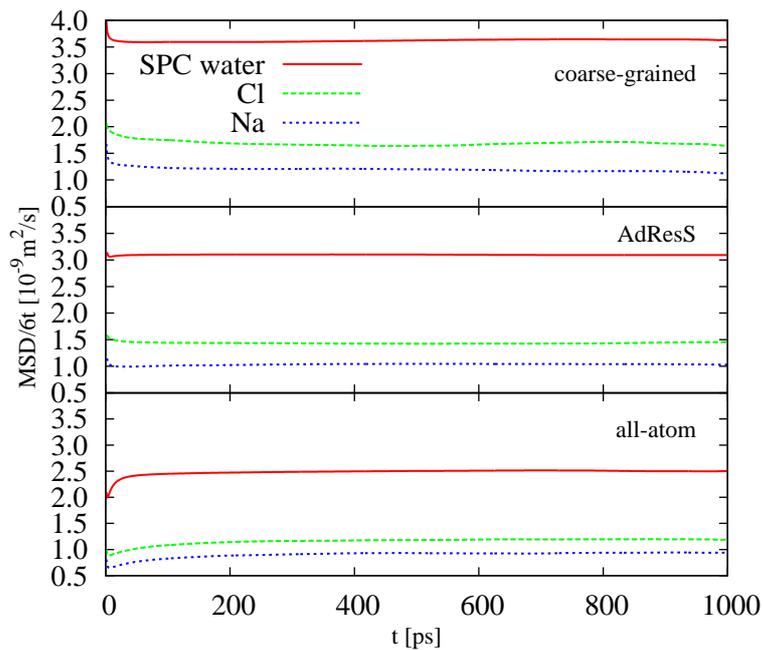


Figure 6: Mean square displacement (MSD) over time plot for all-atom, AdResS and coarse-grained simulations for the system with SPC waters. The plateau values define the corresponding (effective) diffusion constants.

## References

- [1] H. J. C. Berendsen, J. P. M. Postma, W. F. van Gunsteren, and J. Hermans, *Intermolecular Forces*, 331 (1981).
- [2] H. J. C. Berendsen, J. R. Grigera, and T. P. Straatsma, *J. Phys. Chem.* **91**, 6269 (1987).
- [3] S. Bevc, C. Junghans, K. Kremer, and M. Praprotnik, *Original paper*.