EPAPS supplementary information for the JCP article "Simple and Accurate Scheme to Compute Electrostatic Interaction: Zero-dipole Summation Technique for Molecular System and Application to Bulk Water"

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I. PARALLEL COMPUTATIONAL TIMING

Using the TIP3P water system described in the text, we have investigated the parallel timing for calculating the ZD summation method, in comparison with that of the conventional real part of the PME method. We did not use the full part of the PME method, since the evaluation of the Fourier term highly depends on the algorithm and the architecture. The interaction table was constructed using the RESA GC mode with 2 Å buffer length relative to the cutoff length r_c, and updated every 10 time steps.

Table I shows the timing that was averaged over 1000 time steps (discarding several initial step data) for individual methods. The timing of the ZD summation in the practical cutoff range exhibited in the table does not increase much as increasing r_c. The differences between the results of the distinct r_c values tend to be small, as the number of processors increases. As described in the text, we observe that the ZD summation with $\alpha = 0$ has advantages in the accuracies. Such no-damping procedure does not use the error function and so has a gain in view of the timing, as we see that about 2 Å longer r_c can be used, compared with the damping ($\alpha > 0$) cases. Namely, the timing of the ZD summation with $\alpha = 0$ and $r_c = 14$ Å is comparable to that of the ZD summation with $\alpha = 0.1$ and $r_c = 12$ Å, or to that of the real part of the PME method using the cutoff distance of 12 Å; the timing of the ZD summation with $\alpha = 0$ and $r_c = 10$ Å is comparable to that of the real part of the PME method using the cutoff distance of 8 Å, as increasing the number of the processors. Although such parameter dependence can be ignored when one uses the function-tabulation procedure along with a suitable interpolation for potential and force functions, we have the above results in the most simple procedure, which can be used in any architectures.

Table I. Execution time (sec) for 1 step MD simulation of the TIP3P water system by the current ZD summation method and by the real space part of the conventional PME method (RPME). Cutoff length r_c (Å) and damping factor α (Å^{-1}) are indicated; n is the the number of processors.

Method: r_c, α	$n = 8$	$n = 16$	$n = 32$	$n = 64$	$n = 128$
ZD: 10, 0	0.0712	0.0507	0.0410	0.0365	0.0344
ZD: 12, 0	0.0871	0.0587	0.0447	0.0388	0.0361
ZD: 12, 0.1	0.1022	0.0665	0.0492	0.0402	0.0372
ZD: 14, 0	0.1069	0.0767	0.0496	0.0413	0.0389
RPME: 8, 0.35	0.0647	0.0480	0.0388	0.0355	0.0342
RPME: 10, 0.35	0.0802	0.0553	0.0427	0.0371	0.0358
RPME: 12, 0.35	0.1024	0.0661	0.0480	0.0407	0.0364