Supporting Information for "A smooth, non-singular, and faithful discretization scheme for polarizable continuum models: The switching/Gaussian approach"

Adrian W. Lange and John M. Herbert*

1 Switching function

Equations (3.15)–(3.19) in the main paper define the elementary switching function introduced by York and Karplus,[1] which we have adopted for our switching/Gaussian methodology. The parameters $R_{sw,J}$ and α_J (where J indexes atomic spheres) were not completely defined in the paper. These definitions, which we take from Ref. 1, are repeated here for completeness. If N_J is the number of Lebedev grid points used to discretize the Jth sphere, whose radius is R_J, then the width of the switching region around atom J is defined to be

$$R_{sw,J} = R_J \sqrt{\frac{14}{N_J}} \,. \tag{S.1}$$

The scaling parameter α_J is defined as

$$\alpha_J = \frac{1}{2} + \frac{R_J}{R_{sw,J}} - \sqrt{\left(\frac{R_J}{R_{sw,J}}\right)^2 - \frac{1}{28}} \,. \tag{S.2}$$

These two equations complete the definitions of $R_{in,J}$ and $R_{out,J}$, the inner and outer boundaries of the switching region for atom J. Note that the penetration depth, d_{iJ}, which we defined in Eq. (3.17), is the same quantity that York and Karplus denote by $\hat{r}_{iJ}$.

---

*herbert@chemistry.ohio-state.edu

2 Convergence data

Figures 4 and 5 in the paper depict various tests of convergence with respect to the number of Lebedev grid points per atomic sphere, N. (We use the same N_J for all J.) It may be useful to see the actual numerical data, in order to get a sense of the error associated with a particular value of N. Table I provides these data. (Recall that the data set consists of the 20 amino acids.)

References

[1] D. M. York and M. Karplus, J. Phys. Chem. A **103**, 11060 (1999).

N	Δ_{rot}/ 10^{-3} kcal mol^{-1}	$(W_N - W_{1202})$/ kcal mol^{-1}	gradient RMSE/ 10^{-5} a.u.	Δ_{GL}/ 10^{-3} a.u.
		AMBER		
26	61.87 (35.89)	1.6756 (0.6537)	21.24 (5.21)	12.09 (12.26)
50	27.27 (19.66)	0.7744 (0.2865)	11.01 (2.58)	5.37 (5.59)
110	16.86 (0.89)	0.3556 (0.1270)	5.63 (1.32)	2.03 (2.36)
194	8.29 (3.61)	0.1976 (0.0662)	3.75 (0.74)	1.08 (1.26)
302	2.87 (1.52)	0.1259 (0.0423)	2.19 (0.54)	0.67 (0.79)
434	3.18 (2.85)	0.0790 (0.0267)	1.39 (0.36)	0.45 (0.54)
590	2.26 (1.63)	0.0471 (0.0157)	1.04 (0.32)	0.32 (0.39)
770	2.21 (0.44)	0.0236 (0.0087)	0.78 (0.24)	0.24 (0.28)
974	1.76 (0.74)	0.0113 (0.0042)	0.75 (0.21)	0.19 (0.23)
1202	1.54 (0.38)	—	—	0.15 (0.18)
		HF/6-31+G*		
26	99.69 (81.20)	3.0167 (0.6767)	56.11 (6.10)	—
50	61.52 (49.07)	1.7971 (0.4032)	34.55 (5.85)	—
110	33.58 (9.91)	0.7657 (0.1757)	17.34 (2.92)	—
194	14.72 (3.73)	0.4458 (0.1073)	9.97 (2.01)	—
302	16.56 (5.49)	0.2579 (0.0651)	7.31 (1.08)	—
434	4.39 (11.28)	0.1615 (0.0432)	5.10 (1.31)	—
590	6.17 (4.44)	0.0936 (0.0252)	4.28 (1.17)	—
770	3.46 (3.14)	0.0444 (0.0132)	3.55 (0.97)	—
974	4.22 (1.25)	0.0193 (0.0106)	3.35 (0.86)	—
1202	2.55 (1.13)	—	—	—

Table S1: Mean values of the rotational variance (Δ_{rot}), energy and gradient discretization errors, and Gauss' Law error (Δ_{GL}), as a function of the number of Lebedev grid points per atom. Values in parentheses are standard deviations over the set of 20 amino acids. The Gauss' Law error is not computed for the Hartree-Fock (HF) calculations, since not all of the solute charge is contained within the cavity. In evaluating the energy and gradient discretization errors, the result with $N = 1202$ is taken to represent the exact result.