Variational and cavity-free approach to solvation in a multiresolution analysis framework

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Most chemical systems of interest are in solution. Solvent models are therefore an important component of every quantum chemistry software. We successfully implemented a Self Consistent Reaction Field (SCRF) procedure for solving the Generalized Poisson Equation (GPE),

$$\nabla \left[\epsilon(\mathbf{r})\nabla V(\mathbf{r})\right] = -4\pi\rho(\mathbf{r}), \tag{1}$$

for a solvated system using a MW basis as outlined by Fosso-Tande and Harrison (2013). The dielectric function, $\epsilon(\mathbf{r})$, is defined as a functional of a cavity function which describes the values of the permitivity inside, outside and on the surface of the molecular cavity with a convenient sigmoidal shape.
We have also combined the GPE solver with the variational formulation of Lipparini et al.(2010). Our preliminary results look promising in terms of efficiency of the algorithm compared to a more traditional, nested SCRF approach.
This work is part of the ongoing development of MRChem: a multiwavelet code for all-electron DFT calculations

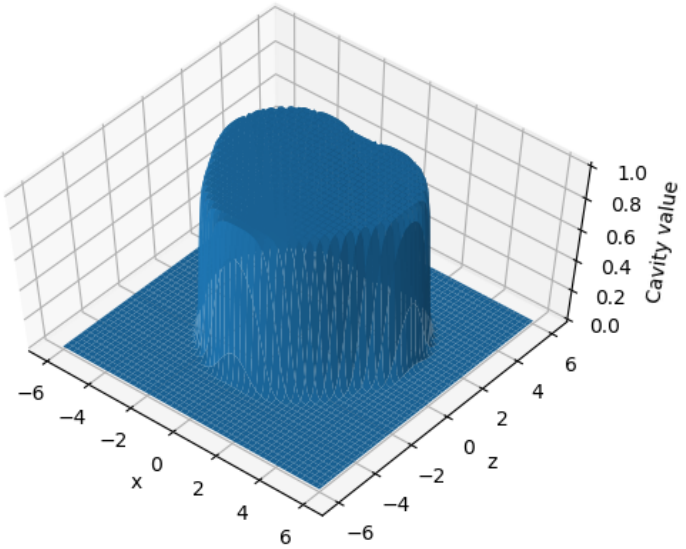

Figure 1: xz-section of a water cavity function. The z axis shows the function value $C = 0$ outside the cavity and $C = 1$ inside the cavity.

References

1. Fosso-Tande J. and Harrison R. J., *Chem. Phys. Lett* **561-562** (2013), 179-184.
2. Lipparini F. et al., *J Chem Phys* **133** (2010), 014106.
3. MRChem, https://github.com/MRChemSoft/mrchem, (2019)