ENHANCING PREDICTIVE ACCURACY IN MOLECULAR ELECTROSTATICS: COUPLING FINITE AND BOUNDARY ELEMENTS WITH VARIABLE PERMITTIVITY

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ABSTRACT. In the domain of molecular biophysics, electrostatic interactions hold a pivotal role in diverse applications, ranging from the analysis of molecular interactions to drug design. Calculating solvation and binding energies is a common practice in these studies, often facilitated by continuous models that simplify complex molecular structures and computational costs. These models delineate the domain into two regions, the solute and solvent, separated by an interface, and apply the Poisson-Boltzmann equation across these regions.

However, a challenge arises when accurately representing the region proximate to the solute-solvent interface, where the constant permittivity description employed by the boundary element method, which we use, may falter in capturing the intricacies of the electrostatic field.

In response to this challenge, we present an innovative approach that couples finite and boundary elements while incorporating variable permittivities. Instead of abrupt changes in permittivity, we introduce a refined technique aimed at smoothing the transition zone. This approach enables us to enhance predictive accuracy in molecular electrostatics.

Computational implementation of this method is realized using state-of-the-art software tools such as Dolfin and Bempp, facilitating the seamless integration of finite and boundary elements.

Our results demonstrate significant improvements in predictive accuracy, particularly in the calculation of solvation and binding energies. We compare our findings with established datasets, underscoring the superior predictive capabilities of our approach.

In conclusion, our work offers a promising avenue for advancing predictive accuracy in molecular electrostatics. By coupling finite and boundary elements with variable permittivity, we mitigate the limitations of existing models and provide a valuable tool for researchers in the field. Our participation in this conference seeks to foster discussion and collaboration, opening doors to further refinement and broader applications of this innovative approach.

Keywords: BEM, FEM, Poisson-Boltzmann, Molecular electrostatics.

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