BRIDGING BOUNDARIES IN MOLECULAR ELECTROSTATICS: TOWARDS LEVERAGING BEM-BASED TOOLS INTO SCIENTIFIC COMMUNITIES

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Abstract. In the domain of computational chemistry, the Poisson-Boltzmann equation stands as a pillar for understanding the electrostatic properties of biomolecules immersed in aqueous environments. Our work explores into the application of the Boundary Element Method (BEM) to solve this equation, offering a precise and versatile numerical framework. This presentation elucidates the unique advantages of BEM in this context, highlighting its accuracy describing the molecular geometry and charges, and treatment of boundary conditions at infinity, and also its limitations in terms of the linear approximation and variation of material parameters in space.

We go beyond the theoretical foundations to discuss practical applications where the boundary integral representation of equations provides a significant advantage over alternative methods. However, our journey does not end with mathematical rigor; it extends into the realm of software development. We introduce the Poisson-Boltzmann & Jupyter (PBJ) code as evidence to our commitment to building robust, sustainable, and user-friendly numerical tools. We stress the importance of making these advanced tools accessible to the computational chemistry community, recognizing that the path to community adoption is fraught with challenges.

Join us in exploring the boundaries of molecular electrostatics, where mathematics, software development, and community engagement converge in pursuit of a common goal: advancing our understanding of the intricate world of biomolecular interactions.

Keywords: boundary element method, Poisson-Boltzmann, molecular electrostatics, Jupyter

Mathematics Subject Classifications (2010): 92E10, 92C40, 45A05

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