Solving The Poisson-Boltzmann Equation With Mimetic Differences

The nonlinear Poisson-Boltzmann equation (PBE) is a fundamental equation widely used to describe the spatial distribution of electrostatic potential, u(r), arising from a molecule or biological macromolecule in electrolyte solutions. This equation is derived from the classical Poisson equation that determines the electrostatic potential arising from a charge distribution within a region, and the Boltzmann distribution that describes how charged particles (e.g., ions) are distributed in the environment. This study aims to obtain the numerical solution to the nonlinear PBE in 2D using mimetic differences, as implemented in the Mimetic Operator Library Enhanced (MOLE). The mimetic PBE solver was tested on simple planar molecules (H_2O, HCl, SO_3, and HCN) represented by atomic point charges derived from quantum chemistry calculations. The visualizations of the electrostatic potentials obtained demonstrate a clear correlation between the signs of the atomic partial charges and the corresponding peaks: negative peaks align with negatively charged atoms, whereas positive peaks are centered on positively charged atoms. The height of the peaks reflects the magnitudes of the charges. These findings validate the mimetic nonlinear PBE solver and hold the potential to significantly impact multiple fields, including computational chemistry and biophysics, once extended to 3D and scenarios with continuous charge distributions.

Luna Huynh, *Yuezhi Mao and Miguel Dumett*

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Poisson-Boltzmann Equation

$$-\nabla \cdot (\varepsilon(\mathbf{r})\nabla u(\mathbf{r})) + \bar{\kappa}^2(\mathbf{r})\sinh(u(\mathbf{r})) = \left(\frac{4\pi e_c^2}{k_B T}\right)\sum_{i=1}^{N_m} z_i \delta(\mathbf{r} - \mathbf{r}_i) \quad \text{in } \Omega \subset \mathbb{R}^2$$

where

$\varepsilon(\mathbf{r})$ is the dimensionless dielectric constant function,
$\bar{\kappa}(\mathbf{r})$ is the modified Debye-Hückel parameter (modified to be dielectric-independent),
e_c is the charge of electron constant,
k_B is Boltzmann's constant,
T is the absolute temperature,
z_i is the partial charge for each atom in a molecule.

Poisson-Boltzmann Equation in Mimetic Differences

$$-D(E \cdot (GU)) + K\sinh(U) = \rho$$

where $E = \text{diag}(\varepsilon)$, $K = \text{diag}(\bar{\kappa}^2)$.

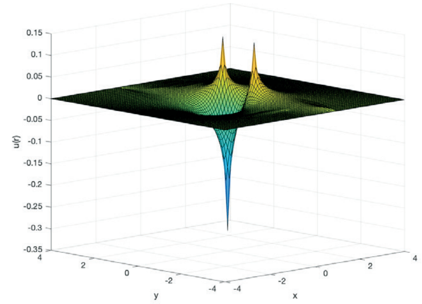

Figure 1: Distribution of electrostatic potential around H_2O. The PBE is solved within domain $\Omega_s = [-4,4] \times [-4,4]$ and $\Omega_m = \{(x,y);\ x^2 + y^2 \le 2\}$.

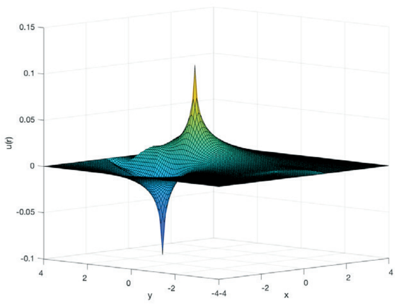

Figure 2: Distribution of electrostatic potential around HCl. The PBE is solved within domain $\Omega_s = [-4,4] \times [-4,4]$ and $\Omega_m = \{(x,y);\ x^2 + y^2 \le 2\}$.

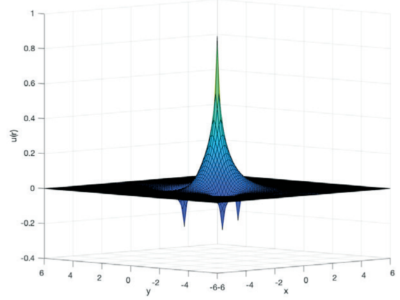

Figure 3: Distribution of electrostatic potential around SO_3. The PBE is solved within domain $\Omega_s = [-6,6] \times [-6,6]$ and $\Omega_m = \{(x,y);\ x^2 + y^2 \le 3\}$.

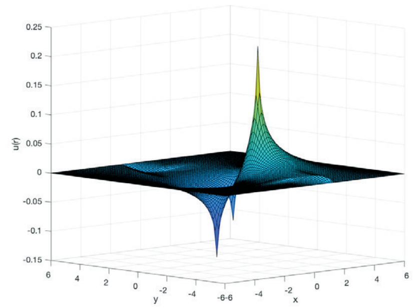

Figure 4: Distribution of electrostatic potential around HCN. The PBE is solved within domain $\Omega_s = [-6,6] \times [-6,6]$ and $\Omega_m = \{(x,y);\ x^2 + y^2 \le 3\}$.