SOLVING THE POISSON-BOLTZMANN EQUATION FOR MACROMOLECULES IN POLARIZABLE MEDIA USING (XPINNS) EXTENDED PHYSICS INFORMED NEURAL NETWORKS

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Abstract. The Poisson-Boltzmann Equation (PBE) serves as a fundamental tool for modeling electrostatic interactions in macromolecular systems immersed in polarizable media, underpinning various biophysical and chemical processes. In this investigation, we leverage the power of Extended Physics Informed Neural Networks (XPINNs) to approximate the electrostatic potential in these scenarios.

Our computational framework employs two distinct Neural Networks—Fully Connected Neural Networks (FCNNs) or Residual Networks (ResNet)—dedicated to different domains: the solute and solvent regions. We also ensure continuity between the two networks through interface conditions on the molecular surface.

This study explores multiple dimensions of our computational approach. We investigate hyperparameter combinations to optimize the accuracy and performance of XPINNs. Additionally, we explore convergence by implementing a self-adapting weighting scheme for loss terms, and a preconditioner loss term, within our XPINN architecture.

While our current model demonstrates success with spherical molecules with a single point charge, our goal for this conference is to extend its applicability to realistic molecular geometries. This is challenging because of the complex interface between the solute and solvent, and the presence of multiple point charges. This progress represents a significant step towards aiding numerical simulations of the electrostatics of macromolecules with machine learning.

Keywords: XPINNs, Physics Informed Neural Networks, Poisson-Boltzmann Equation.

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