# Solving Green's function using neural networks to model electrostatic correlations

*Nikhil Agrawal* *CHEM247 Spring 2022: Final Project proposal*

The study of electrical double layer resulting from a charged surface is at the heart of colloidal and interfacial sciences. However, the standard mean-field PB theory fails to describe systems with large surface-charge density, high counter-ion valency and high ion concentration because it ignores the electrostatic correlation. To model ion-ion correlations phenomena one has to go beyond mean-field level and include fluctuations in the theory. For this a Gaussian Renormalized Fluctuation theory was given by Zhen-Gang Wang at Caltech. One of the key equations in this theory for symmetric planar systems is

$$\mathcal{L}G(z,z) = -\frac{\partial^2 G(s,z,z')}{\partial z^2} + s^2(z)G(s,z,z') = \frac{\delta(z,z')}{\epsilon} \tag{1}$$

where $\epsilon$ is the dielectric constant of the system, $s$ is a smooth function and $G$ is the Green's function we want to solve for. The aim of this project will be to use artificial neural networks (ANN) to approximate the function $G$ in [0,L]. The following boundary conditions (BC) for regions $z < 0, z' \geq 0$ and $z > L, z' \leq L$ respectively will be used:

$$\frac{\partial G(s,z,z')}{\partial z'} = s(z=0)G(s,z,z') \tag{2}$$

$$\frac{\partial G(s,z,z')}{\partial z'} = -s(z=L)G(s,z,z') \tag{3}$$

Existing finite difference methods to solve for the above problem become very complex and inefficient for the three dimensional analog of the Equation 1. Solving these three-dimensional PDE is very important if we want to solve for ion-ion correlations in asymmetric systems. Through this project I aim to see the capabilities of the machine learning framework to solve for such two point correlation functions.

I have decided to divide the project into two parts. The first half will involve solving Equation 1 for the case when $s(z) =$ constant. In this case there is an analytical solution to the PDE given by

$$G(s,z,z') = \frac{e^{-s|z-z'|}}{2s\epsilon} \tag{4}$$

Using this analytical solution as my labelled data I will use a supervised learning approach on a fully connected neural network to finalize the architecture of the network. I will use a suitable random number generator to create a big enough sample data set for $(z, z')$. Let's call the neural network for this case to be $NN_1(z,z)$ which satisfies $NN_1(z,z) = G(z, z\text{''}, s(z) = constant)$.

In the second half of the project using the architecture of $NN_1$, I will try to train a new neural network, $NN_2$, which will replicate the function $G(z, z, s(z))$ when $s(z)$ is not a constant. I am planning to use a simple linear or tanh type function for $s(z)$. To train the network I we will use Equations 1,2 and 3 to write a mean-square error type loss function. The derivataives of $G$ or $NN_2$ with respect to $z$ can be calculated using automatic differentiation tools of Pytorch. The singularity associated with the dirac delta function can be approximated using a continuous Gaussian density function with variance tending to zero. Fortunately, there has been some work on a similar problem before from which I plan to borrow some ideas (Teng et al. 2021, arXiv:2105.11045v1). Another piece of literature on which I will rely upon is the pioneering work on Physics Inspired Neural Networks by M. Raissi et al. 2019.