WONAPDE 2024

SEVENTH CHILEAN WORKSHOP ON NUMERICAL ANALYSIS OF PARTIAL DIFFERENTIAL EQUATIONS

UNIVERSIDAD DE CONCEPCIÓN, CONCEPCIÓN, CHILE

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UNIVERSIDAD TECNICA FEDERICO SANTA MARIA

Agencia Nacional de Investigación y Desarrollo

XPINN Solver for 3D Poisson-Boltzmann Equation

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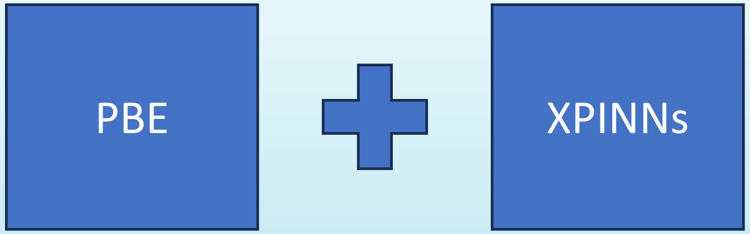
Introduction

The aim is to solve the Poisson-Boltzmann equation using the *Extended Physics Informed Neural Networks* technology.

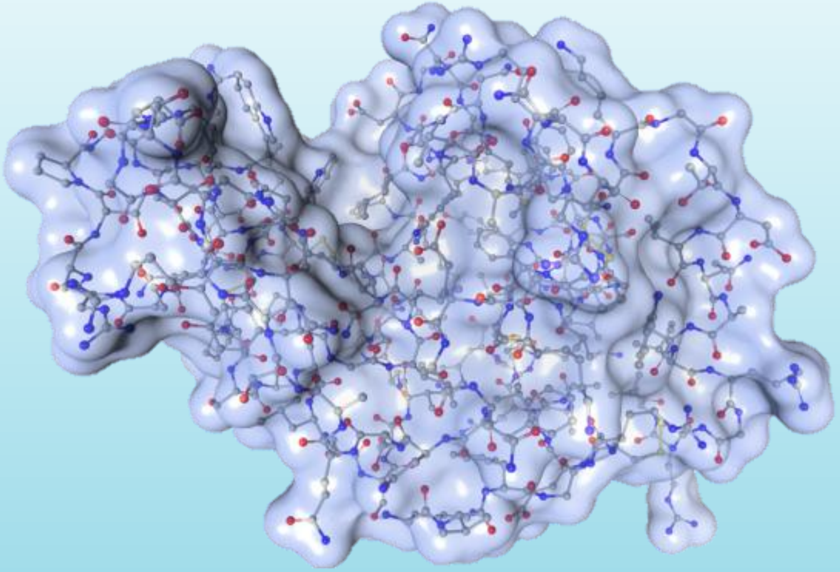
- Poisson-Boltzmann Equation: Models the interaction of macromolecules in a polarizable media.
- PINNs: Physics Informed Neural Networks. Method used to solve PDEs.



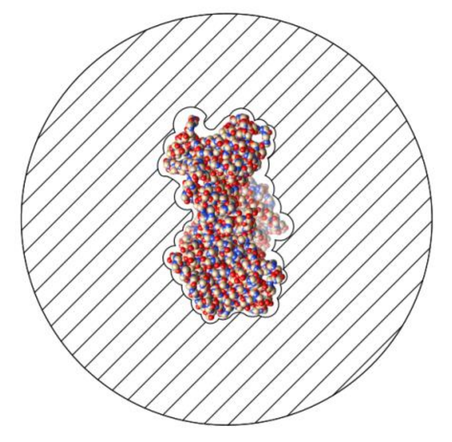
- New Implementation.
- Usable in real-world applications.
- Biochemistry.

Considerations:

- 3D problem.
- 2 domains (solute and solvent region).
- A lot of loss terms needed, and some optional can be added.

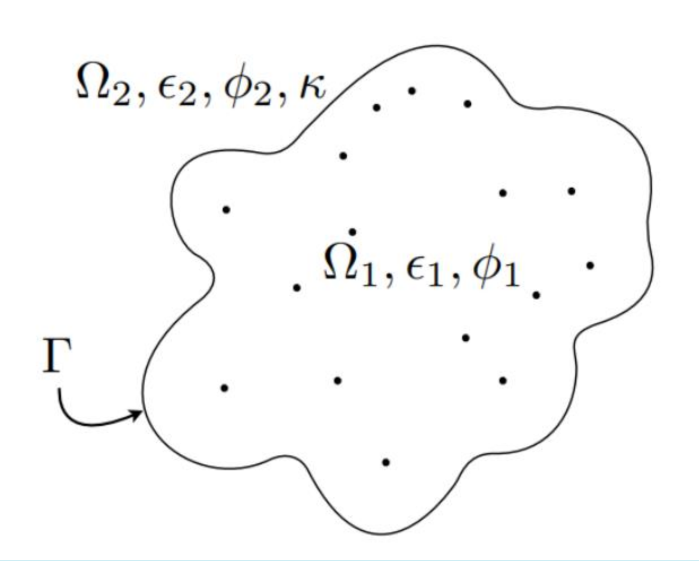


Poisson-Boltzmann Equation



- Applicable to macromolecules in a polarizable media.
- Obtained using the Implicit Solvent Method.

$$\begin{cases} \nabla^2 \phi_1 = -\dfrac{1}{\epsilon_1} \displaystyle\sum_k q_k \delta(\mathbf{x} - \mathbf{x}_k) & \mathbf{x} \in \Omega_1 \\ \nabla^2 \phi_2 = \dfrac{2c^\infty q_e}{\epsilon_2} \sinh\left(\dfrac{\phi_2 q_e}{k_b T}\right) & \mathbf{x} \in \Omega_2 \end{cases}$$

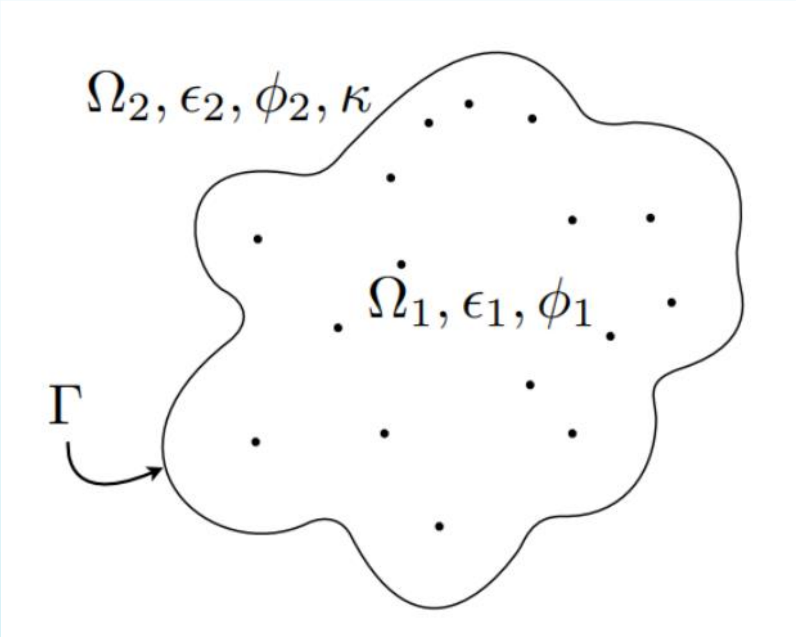


Linearized: $\nabla^2 \phi_2 = \kappa^2 \phi_2$ $\quad \kappa^2 = \dfrac{2c^\infty q_e^2}{\epsilon_2 k_b T}$

Poisson-Boltzmann Equation

- Interface conditions:

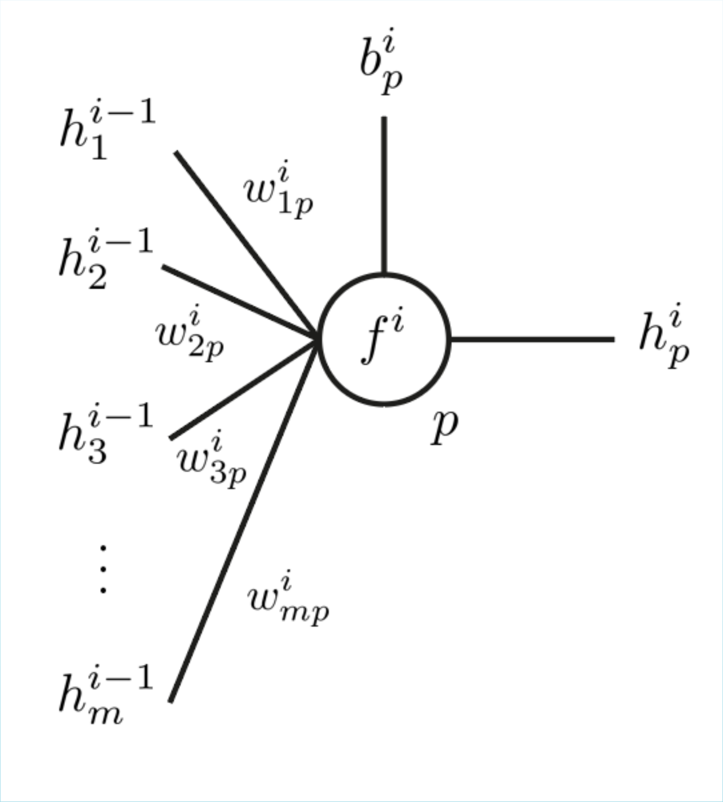
$$\begin{cases} \phi_1 = \phi_2 & \mathbf{x} \in \Gamma \\ \epsilon_1 \dfrac{\partial \phi_1}{\partial n} = \epsilon_2 \dfrac{\partial \phi_2}{\partial n} & \mathbf{x} \in \Gamma \end{cases}$$



Artificial Neural Networks (ANN)

- Operations in every perceptron (neuron).
- Considering the p-th perceptron of the i-th layer:

It has weights in the conexions w^i_{mp}, bias b^i_p, and activation function f^i.



$$h^i_p = f^i\left(\sum_{j=1}^{m} h^{i-1}_j w^i_{jp} + b^i_p\right)$$

Artificial Neural Networks (ANN)

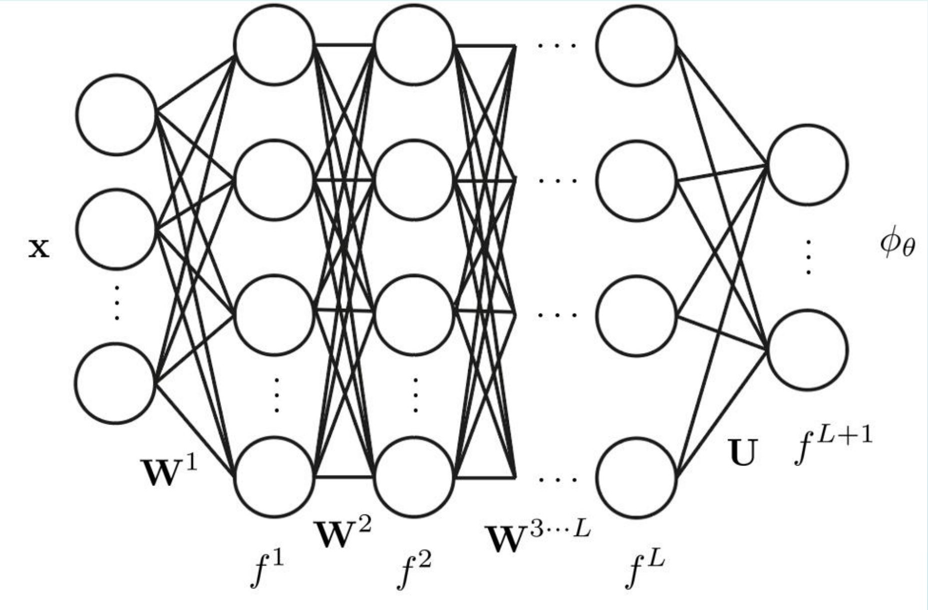
- Assembling multiple interconnected perceptrons forms an Artificial Neural Network (ANN).

$$\phi_\theta = \mathcal{N}(\mathbf{x};\theta)$$

- Example: *Fully Connected Neural Network*

$$\theta = \{\boldsymbol{W}^1, \boldsymbol{b}^1, \ldots, \boldsymbol{W}^L, \boldsymbol{b}^L, \boldsymbol{U}, \boldsymbol{c}\}$$

$$\begin{cases} \boldsymbol{h}^1 = f^1(\mathbf{x}\boldsymbol{W}^1 + \boldsymbol{b}^1) & i = 1 \text{ capa entrada} \\ \boldsymbol{h}^i = f^i(\boldsymbol{h}^{i-1}\boldsymbol{W}^i + \boldsymbol{b}^i) & 2 \leq i \leq L \text{ capas ocultas} \\ \phi_\theta = f^{L+1}(\boldsymbol{h}^L\boldsymbol{U} + \boldsymbol{c}) & i = L+1 \text{ salida} \end{cases}$$



ANN and PINNs (Physics Informed Neural Networks)

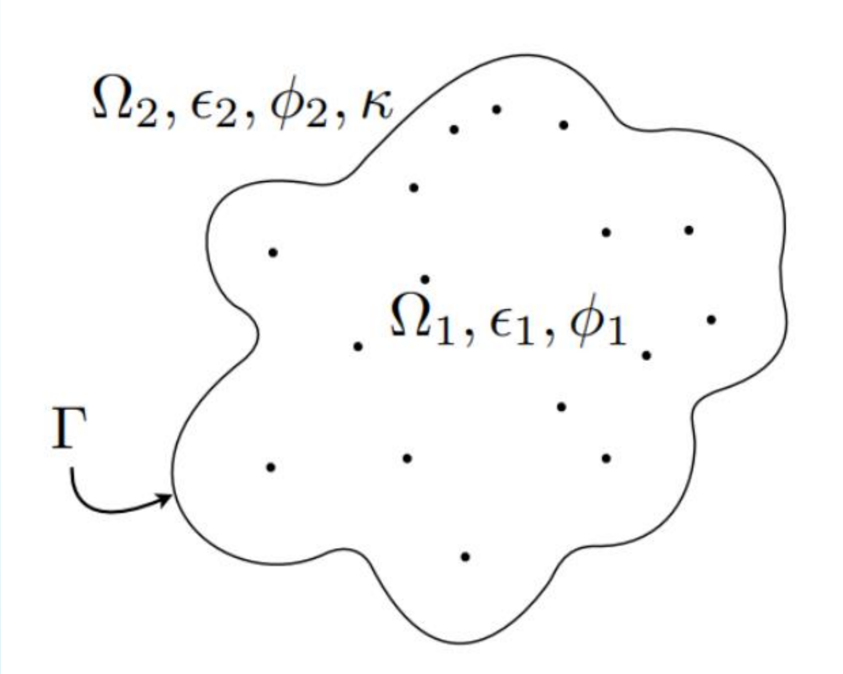
- The concept involves incorporating the equation to solve (residuals, boundary conditions, physics laws, etc.) into the loss function $\mathcal{L}$.
- This ensures that the output of the ANN approximates the solution of the PDE.
- Optimization algorithms based on gradient descent. $\theta^* = \underset{\theta}{\operatorname{argmin}}\, \mathcal{L}(\theta; \mathcal{S})$
- Loss function is evaluated on the $\mathcal{S}$ set (collocation points).
- Algorithms: ADAM, L-BFGS + stochastic methods

$$\theta_{k+1} = \theta_k - \lambda \nabla_\theta \mathcal{L}(\theta_k; \mathcal{S}_j) \qquad \mathcal{S}_j \subset \mathcal{S}$$

XPINN Applied to PBE

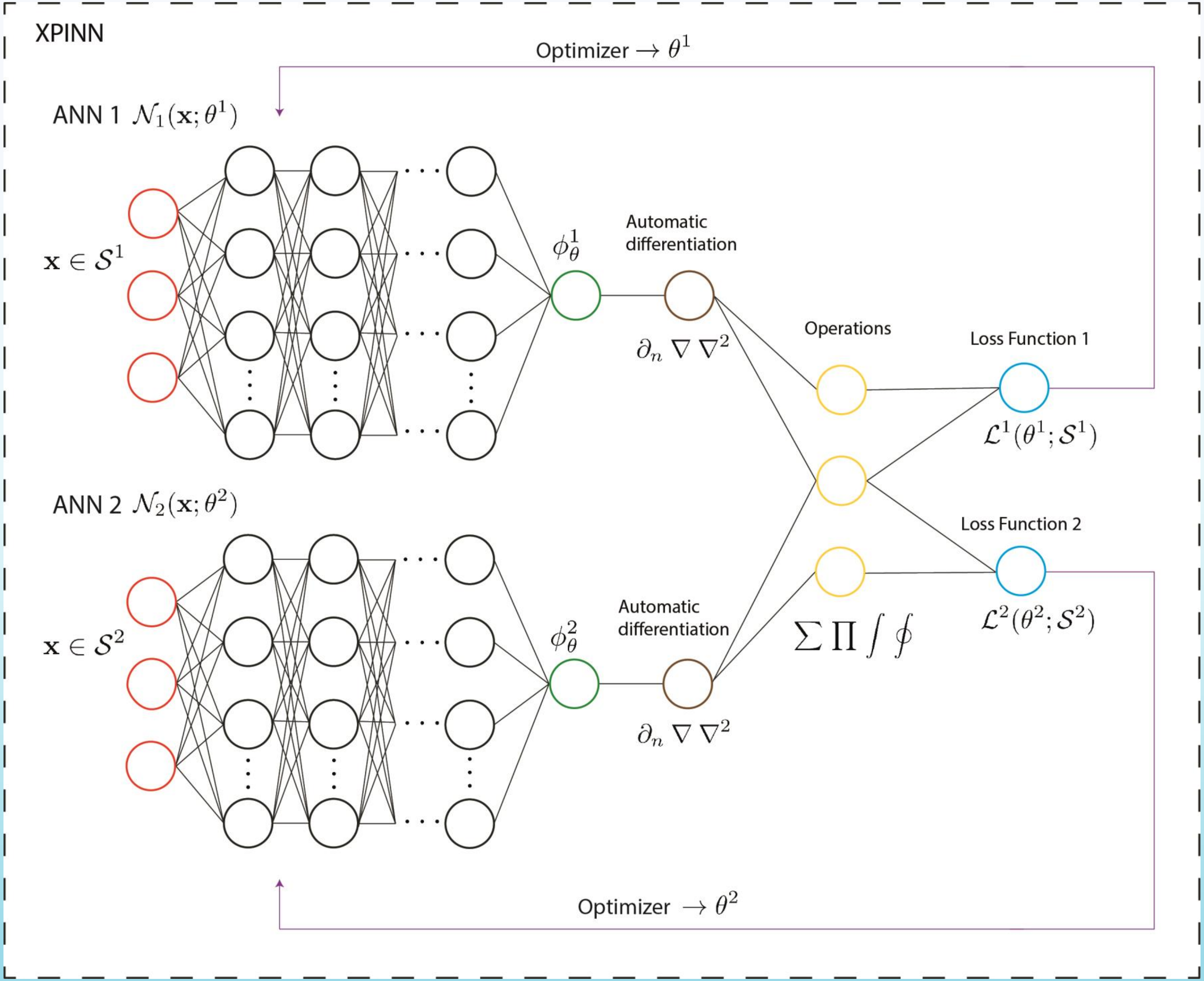
- 2 ANN that outputs the electrostatic potential:
  - N°1: Solute region.
  - N°2: Solvent region.

$$\phi \approx \begin{cases} \phi_\theta^1 = \mathcal{N}_1(\mathbf{x}; \theta^1) & \mathbf{x} \in \Omega_1 \\ \phi_\theta^2 = \mathcal{N}_2(\mathbf{x}; \theta^2) & \mathbf{x} \in \Omega_2 \end{cases}$$



- The loss functions will depend on both ANN, including the following terms:
  - Residual PBE.
  - Boundary conditions.
  - Interface relations.
  - Experimental data.
  - Gauss Law.

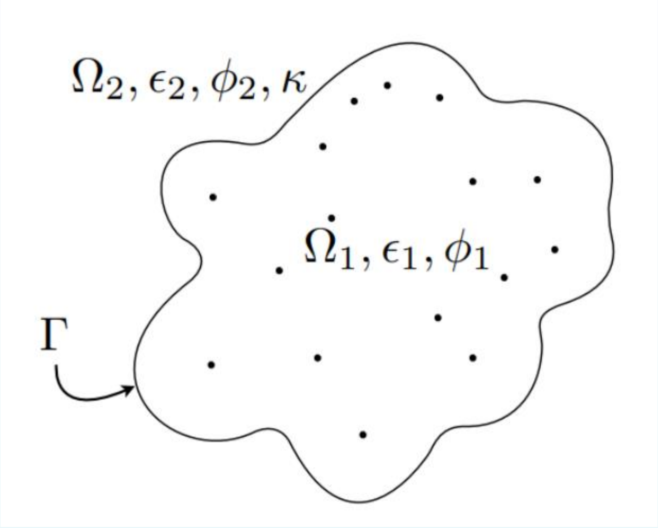
$$\mathcal{L}(\mathcal{S}) = \sum_k w_k \mathcal{L}_k(\mathcal{S}_k)$$



XPINNs for PBE:

- 2 ANN (solute and solvent regions).
- 2 Loss functions that depends on both ANNs.

XPINN Applied to PBE



$$\phi \approx \begin{cases} \phi_\theta^1 = \mathcal{N}_1(\mathbf{x};\theta^1) & \mathbf{x} \in \Omega_1 \\ \phi_\theta^2 = \mathcal{N}_2(\mathbf{x};\theta^2) & \mathbf{x} \in \Omega_2 \end{cases}$$

- Residuals:

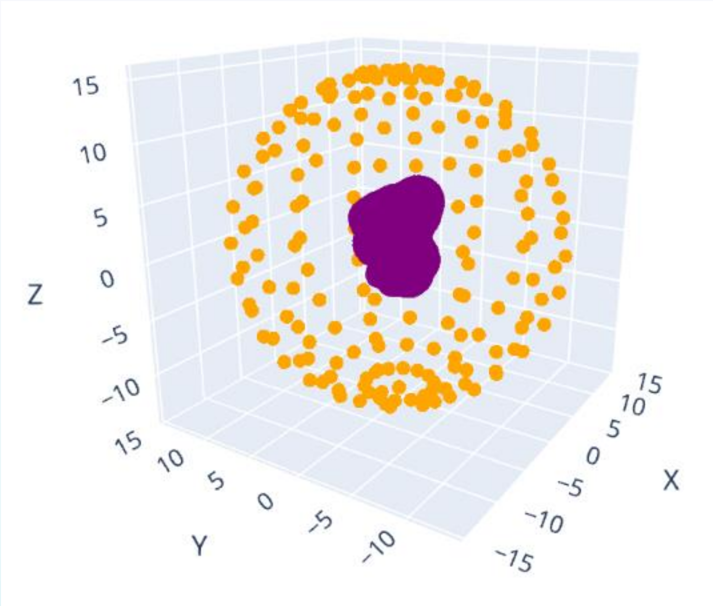
$$\mathcal{L}_{pde}^1(\mathcal{S}_{pde}) = \frac{1}{N_{pde}} \sum_{x_i \in \mathcal{S}_{pde}} \left[\nabla^2 \phi_\theta^1(x_i) + \frac{1}{\epsilon_1} \sum_k q_k \delta(x_i - x_k) \right]^2$$

*Dirac delta will be approximated by a Gaussian function.

$$\mathcal{L}_{pde}^2(\mathcal{S}_{pde}) = \frac{1}{N_{pde}} \sum_{x_i \in \mathcal{S}_{pde}} \left[\nabla^2 \phi_\theta^2(x_i) - \kappa^2 \phi_\theta^2(x_i) \right]^2$$

$$\delta(x) \approx \frac{1}{(2\pi)^{3/2}\sigma^3} e^{-\frac{1}{2\sigma^2}\|x\|^2}$$

XPINN Applied to PBE



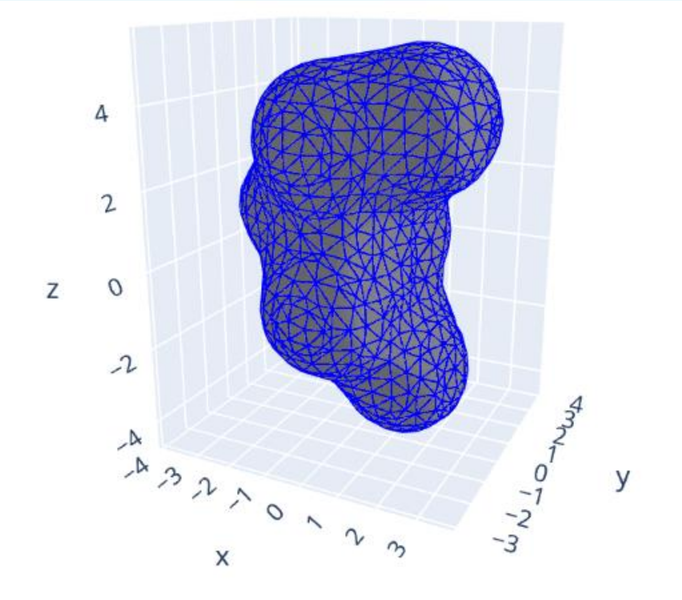
- Boundary condition:

$$\mathcal{L}_{bc}^2(\mathcal{S}_{bc}) = \frac{1}{N_{bc}} \sum_{x_i \in \mathcal{S}_{bc}} \left[\phi_\theta^2(x_i) - \frac{1}{4\pi\epsilon_2} \sum_k \frac{q_k \mathrm{e}^{-\kappa|x_i - x_k|}}{|x_i - x_k|} \right]^2$$

- Interface conditions (j-th ANN)

$$\mathcal{L}_{Iu}^j(\mathcal{S}_I) = \frac{1}{N_I} \sum_{x_i \in \mathcal{S}_I} \left[\phi_\theta^j(x_i) - \overline{\phi}_\theta(x_i) \right]^2$$

$$\mathcal{L}_{Id}^j(\mathcal{S}_I) = \frac{1}{N_I} \sum_{x_i \in \mathcal{S}_I} \left[\epsilon_j \partial_n \phi_\theta^j(x_i) - \overline{\epsilon \partial_n \phi}_\theta(x_i) \right]^2$$



XPINN Applied to PBE

- "Known solution" in random positions (results from software pbj + 10% Noise) (j-th ANN):

$$\mathcal{L}^{j}_{data}(\mathcal{S}_{data}) = \frac{1}{N_{data}} \sum_{x_i \in \mathcal{S}_{data}} \left[\phi^{j}_{\theta}(x_i) - \phi^{*}_{\theta}(x_i) \right]^2$$

- Gauss Law: Additional Physics Law.

$$\mathcal{L}_{Gauss} = \left| \oint_{\Gamma} \overline{\epsilon \partial_n \phi}_{\theta}(x') \, \mathrm{d}S(x') - \sum_{k} q_k \right|^2$$

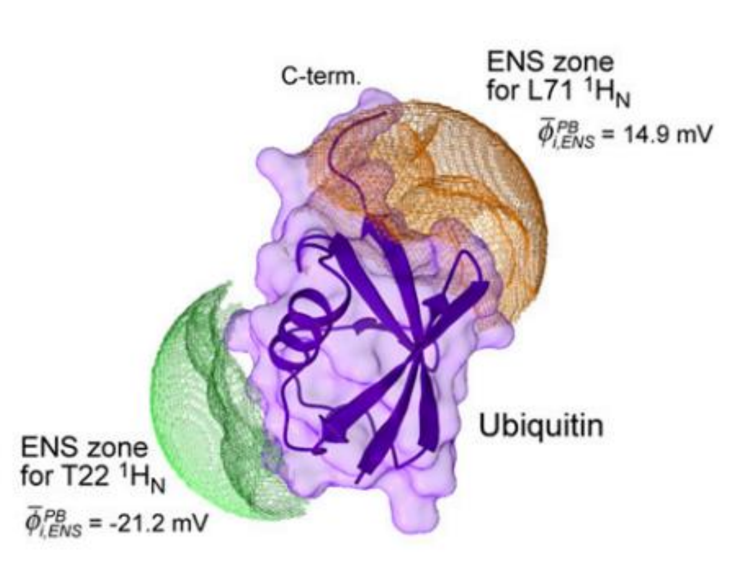
Experimental data ϕ_{ENS}

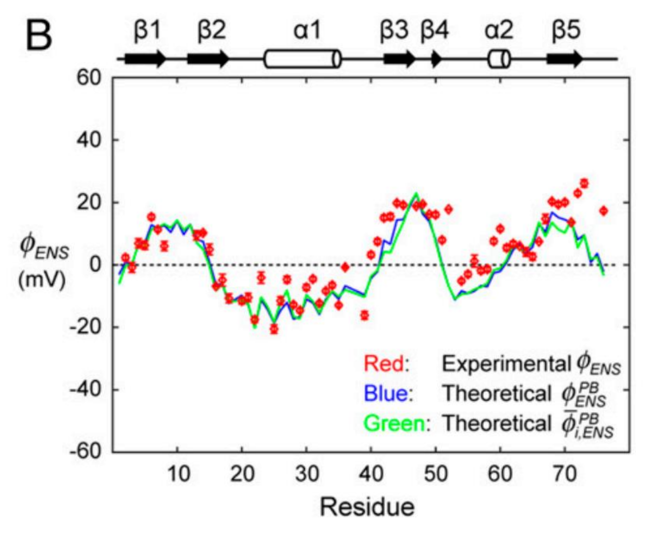
Results for experimental effective near-surface potential.

- For each hydrogen atom h:

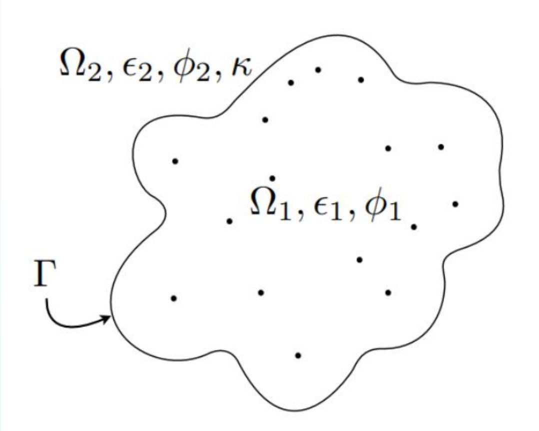
$$\phi_{ENS}(x_h) = \frac{-k_b T}{2q_e} \ln \left(\frac{\int_0^\infty r^{-4}\, \mathrm{e}^{-\frac{q_e \phi_\theta(r)}{k_b T}}\, \mathrm{d}r}{\int_0^\infty r^{-4}\, \mathrm{e}^{\frac{q_e \phi_\theta(r)}{k_b T}}\, \mathrm{d}r} \right)$$

$$\mathcal{L}_E(\mathcal{S}_H) = \frac{1}{N_H} \sum_{x_h \in \mathcal{S}_H} \left[\phi_{ENS,\theta}(x_h) - \phi_{ENS}(x_h) \right]^2$$





Solvation Energy



$$G_{solv} = \frac{1}{2}\sum_k q_k \phi_{reac}(x_k) \qquad \phi_{reac} = \phi - \phi_{coulomb}$$

- Green identities are used for getting the reaction potential at the point charges (uses the potential at interface):

$$\phi_{reac}(x_k) = \frac{1}{4\pi}\oint_\Gamma \overline{\frac{\partial \phi_1}{\partial n}} \frac{1}{|x_k - x'|}\,\mathrm{d}S(x') - \frac{1}{4\pi}\oint_\Gamma \overline{\phi}\frac{\partial}{\partial n}\left(\frac{1}{|x_k - x'|}\right)\mathrm{d}S(x')$$

Weights balancing algortihm for loss terms

- The working principle is to balance the contribution of the different loss terms for the modification of the set θ.

$$\hat{w}_k = \frac{\sum_i \|\nabla_\theta \mathcal{L}_i\|}{\|\nabla_\theta \mathcal{L}_k\|}$$

$$w_{k,\text{new}} = \alpha w_{k,\text{old}} + (1-\alpha)\hat{w}_k$$

- This algorithm works fine, being applied every 1000 or 2000 iterations.

Implementation

- All the simulations were implemented using a full-batch approach, with **~15.000 points** per dataset.
- For the architecture, **FCNN** was preferred, with addition of a **scale layer** and a **Fourier features layer**, after the input layer.

$$y_{fourier} = [\cos(Bx), \sin(Bx)]$$

Where B is a matrix generated by a normal distribution (non trainable), using **256 features**.

- The preferred hyperparameters were: **4 hidden layers with 200 neurons per layer**, with **tanh** as activation function.
- **Exponential decay learning rate** was used, starting from 0,001
- The optimization algorithm used was **ADAM**.

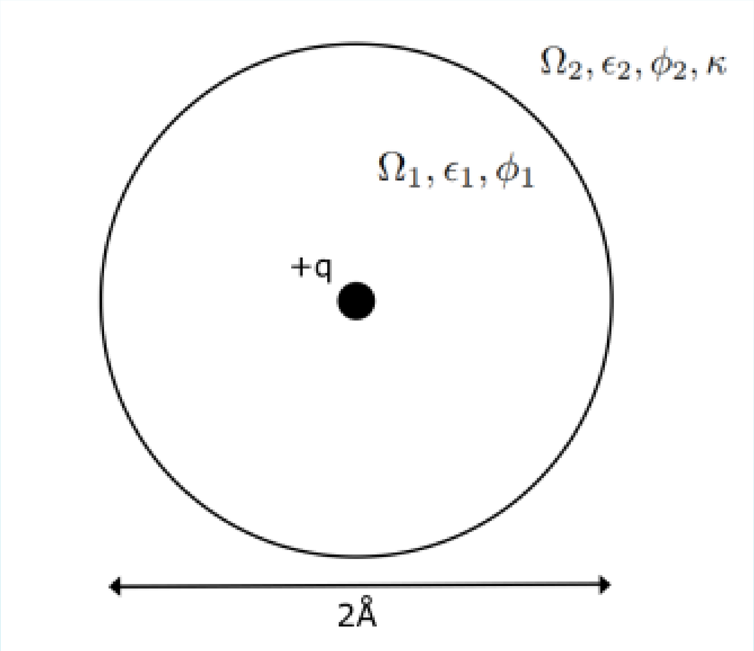
Validation: Born Ion

- Spherical molecule, 1 point charge.
- Analytical solution is known.
- Very simple test case.

$$\phi_1(r) = \frac{q}{4\pi}\left(\frac{1}{\epsilon_1 r} - \frac{1}{\epsilon_1 R} + \frac{1}{\epsilon_2(1+\kappa R)R}\right)$$

$$\phi_2(r) = \frac{q}{4\pi}\frac{\exp(-\kappa(r-R))}{\epsilon_2(1+\kappa R)r}$$

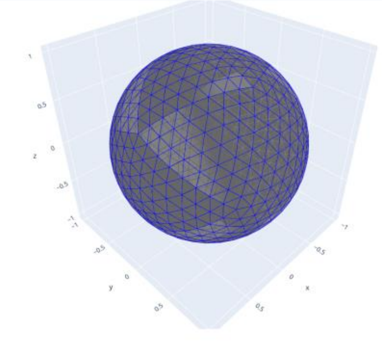
- L2 error at interface can be calculated.



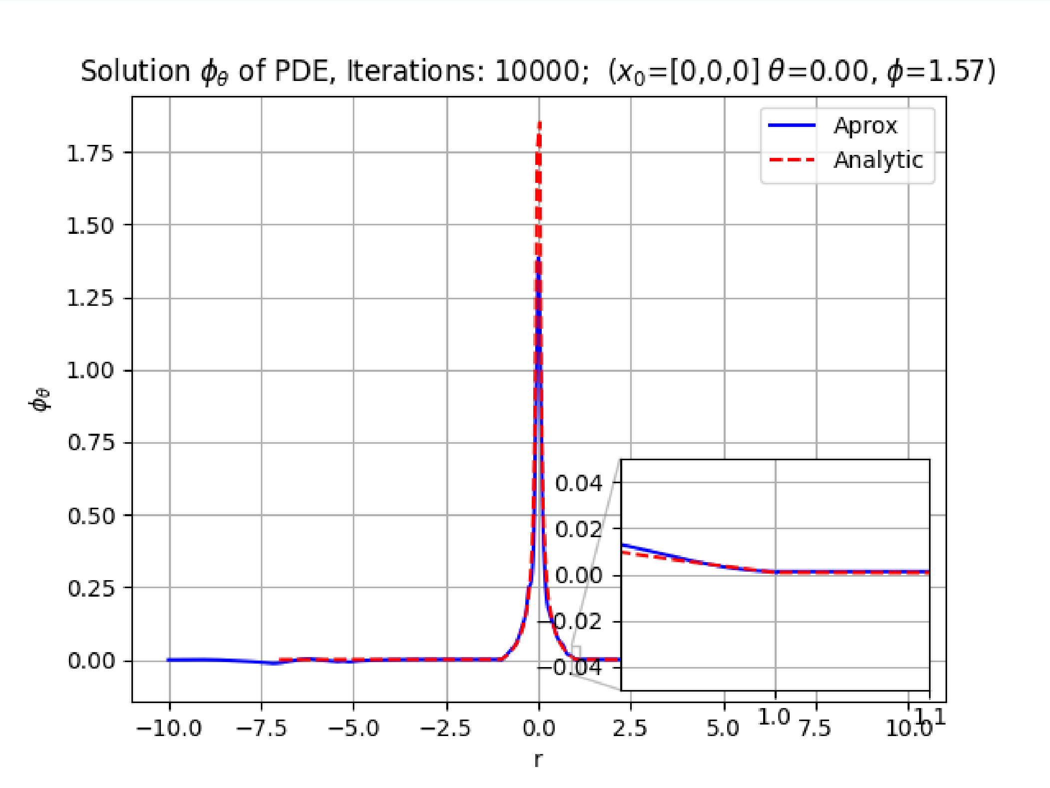
Born Ion

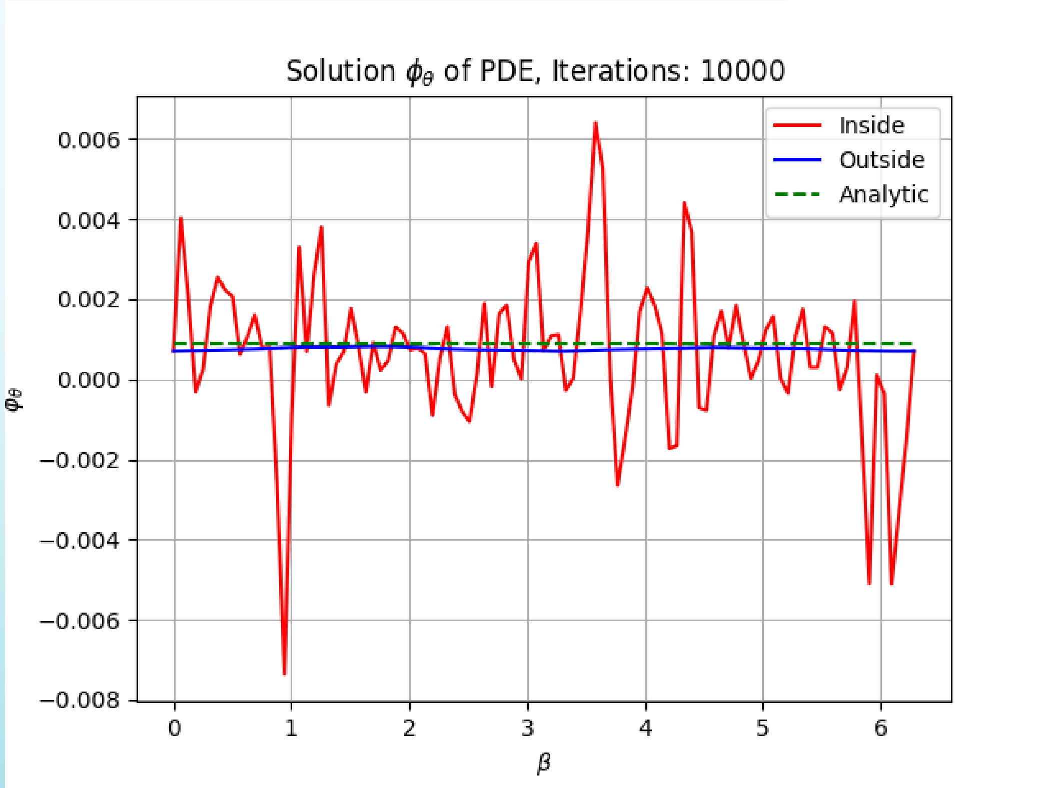
BORN ION			Architecture				Loss terms				Results					
N° Sim	Mesh	ARCH	HL	NpL	F	W	P	K	G	E	Gsolv_value	L2_analytic	L2_cont_u	L2_cont_du	Loss_NN1	Loss_NN2
1	Medium	FCNN	4	200				Noise			-248.181	5.13.E+02	2.13.E-02	1.57.E-02	3.28.E+00	7.80.E-04
2	Medium	FCNN	4	200	I	X		Noise	X		32.485	1.16.E+03	4.02.E-02	8.43.E-02	1.10.E+05	8.83.E-03
3	Medium	FCNN	4	200	I	X		Noise		X	0.712	2.52.E+01	2.76.E-04	7.73.E-04	3.80.E-01	5.47.E+02
4	Medium	FCNN	4	200	I	X		Noise	X	X	30.944	7.24.E+02	2.25.E-02	1.37.E-01	2.62.E-02	7.11.E+02
5	Medium	FCNN	4	200	I	X			X	X	48.058	1.88.E+03	6.20.E-02	2.15.E-01	6.23.E+04	2.37.E+02
6	Medium	FCNN	4	200	I	X	X		X	X	-1.187	4.42.E+01	2.07.E-04	1.43.E-04	1.82.E-04	2.25.E-04
7	Medium	FCNN	4	200	I	X	X	Noise	X	X	4.942	3.06.E+02	1.08.E-02	2.51.E-02	1.18.E-02	2.10.E+02
8	Medium	FCNN	4	200		X	X		X	X	-14.575	2.83.E+02	5.65.E-03	2.64.E-03	2.55.E+00	1.70.E+01
9	Medium	FCNN	4	200	I			Noise	X	X	97.865	2.27.E+03	6.78.E-02	2.02.E-01	5.71.E+01	2.35.E+02
10	Medium	FCNN	4	200	I						38.634	6.20.E+02	1.00.E-02	1.27.E-02	3.01.E-01	2.75.E-04
11	Medium	FCNN	4	200	I	X		Noise			0.406	3.05.E+01	9.71.E-04	2.34.E-03	1.29.E+01	7.00.E-06
12	Medium	FCNN	4	200	I	X		Noise		X	-0.005	2.68.E+01	4.04.E-04	4.02.E-05	2.33.E-01	1.68.E+01
13	Medium	FCNN	4	200	I	X				X	-0.052	1.08.E+02	7.22.E-08	1.35.E-07	7.59.E-09	8.52.E+02
14	Medium	FCNN	4	200	I	X	X			X	-0.672	3.15.E+01	7.58.E-05	2.07.E-05	1.06.E-05	9.16.E-04
15	Medium	FCNN	4	200	I	X	X	Noise		X	-0.411	3.10.E+01	8.43.E-05	1.53.E-04	3.48.E-03	4.47.E+00
16	Medium	FCNN	4	200		X	X			X	-0.359	3.38.E+01	5.38.E-04	1.77.E-04	1.17.E-01	1.60.E+01
17	Medium	FCNN	4	200	I			Noise		X	34.074	1.53.E+03	5.41.E-02	1.82.E-01	9.36.E+01	2.06.E-01
18	Coarse	FCNN	4	200	I	X		Noise		X	-0.502	1.65.E+01	2.15.E-05	6.25.E-05	4.12.E-03	1.45.E+00
19	Fine	FCNN	4	200	I	X		Noise		X	-0.503	6.74.E+01	7.20.E-04	1.32.E-03	1.29.E+00	2.07.E+01
20	Medium	FCNN	4	300	I	X		Noise		X	3.566	7.02.E+02	2.46.E-02	8.48.E-02	1.97.E-02	1.82.E+01
21	Medium	FCNN	4	120	I	X		Noise		X	-0.072	2.66.E+01	1.09.E-04	2.79.E-04	2.35.E-01	7.08.E+01
22	Medium	FCNN	3	200	I	X		Noise		X	-0.241	2.87.E+01	2.32.E-04	2.82.E-05	3.27.E-03	2.96.E+00
23	Medium	FCNN	5	200	I	X		Noise		X	0.126	2.71.E+01	1.59.E-04	3.18.E-05	7.62.E-03	4.15.E+01
24	Medium	FCNN	4	200	B	X		Noise		X	-33.431	7.70.E+00	1.51.E-04	7.12.E-05	7.76.E-05	7.79.E-05
25	Medium	FCNN	4	200		X		Noise		X	8.756	1.84.E+02	6.92.E-03	3.55.E-04	1.98.E+01	1.75.E+02
26	Medium	ResNet	4	200	I	X		Noise		X	-0.126	5.41.E+01	1.74.E-03	3.46.E-03	2.50.E+00	1.70.E+02
27	Medium	ResNet	4	200	B	X		Noise		X	-14.593	8.40.E+02	2.93.E-02	8.42.E-03	2.34.E-01	1.03.E+01
28	Medium	ResNet	4	200		X		Noise		X	10.164	3.88.E+02	2.83.E-03	2.85.E-04	7.95.E+00	4.57.E+02
29	Coarse	FCNN	4	200	B	X		Noise		X	-43.004	1.38.E+02	2.41.E-04	1.64.E-05	2.07.E-05	5.94.E+01
30	Fine	FCNN	4	200	B	X		Noise		X	13.165	3.49.E+02	1.81.E-03	1.85.E-03	4.89.E-02	6.76.E+02
31	Medium	FCNN	4	300	B	X		Noise		X	4.579	1.06.E+03	3.23.E-02	1.42.E-01	9.39.E+02	1.08.E+02
32	Medium	FCNN	4	120	B	X		Noise		X	-41.351	6.16.E+00	1.41.E-04	5.21.E-04	5.33.E+00	1.66.E-04
33	Medium	FCNN	3	200	B	X		Noise		X	-18.919	2.86.E+02	4.60.E-03	9.48.E-03	1.49.E+01	7.85.E+00
34	Medium	FCNN	5	200	B	X		Noise		X	249.467	1.21.E+03	3.34.E-02	8.27.E-03	1.02.E-01	1.87.E+02

Born Ion

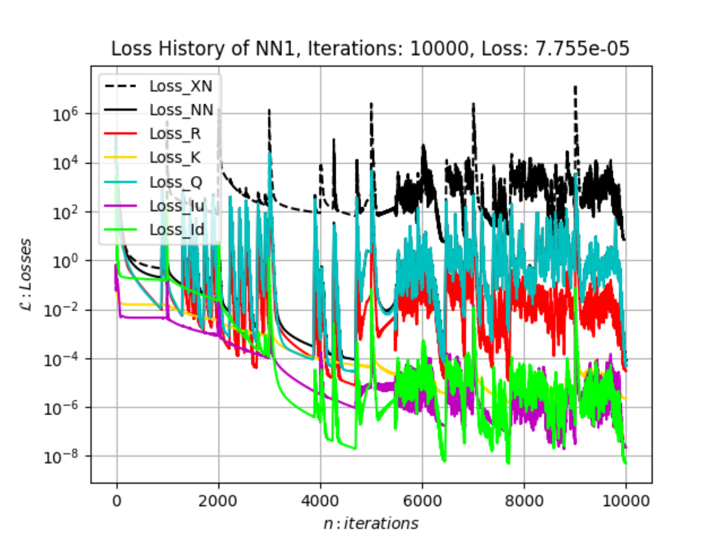


For 10.000 iterations, it “converges” to the analytical solution.

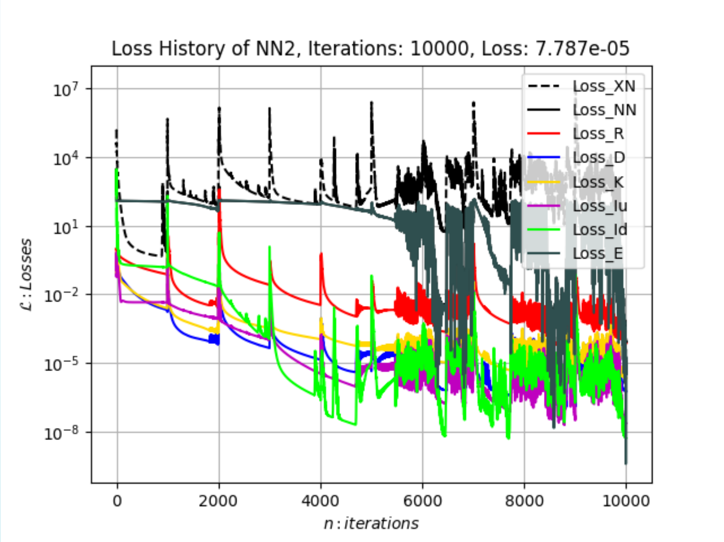




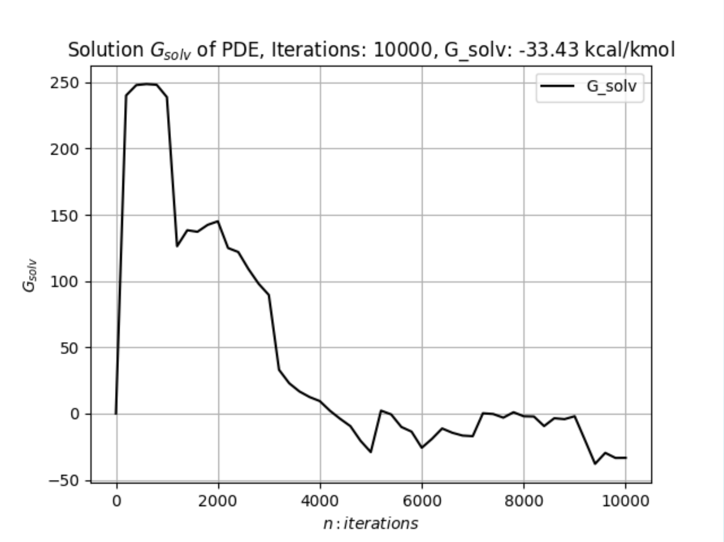
Born Ion



Loss History of NN1, Iterations: 10000, Loss: 7.755e-05
Loss_XN
Loss_NN
Loss_R
Loss_K
Loss_Q
Loss_Iu
Loss_Id
$\mathcal{L}: Losses$
$n: iterations$

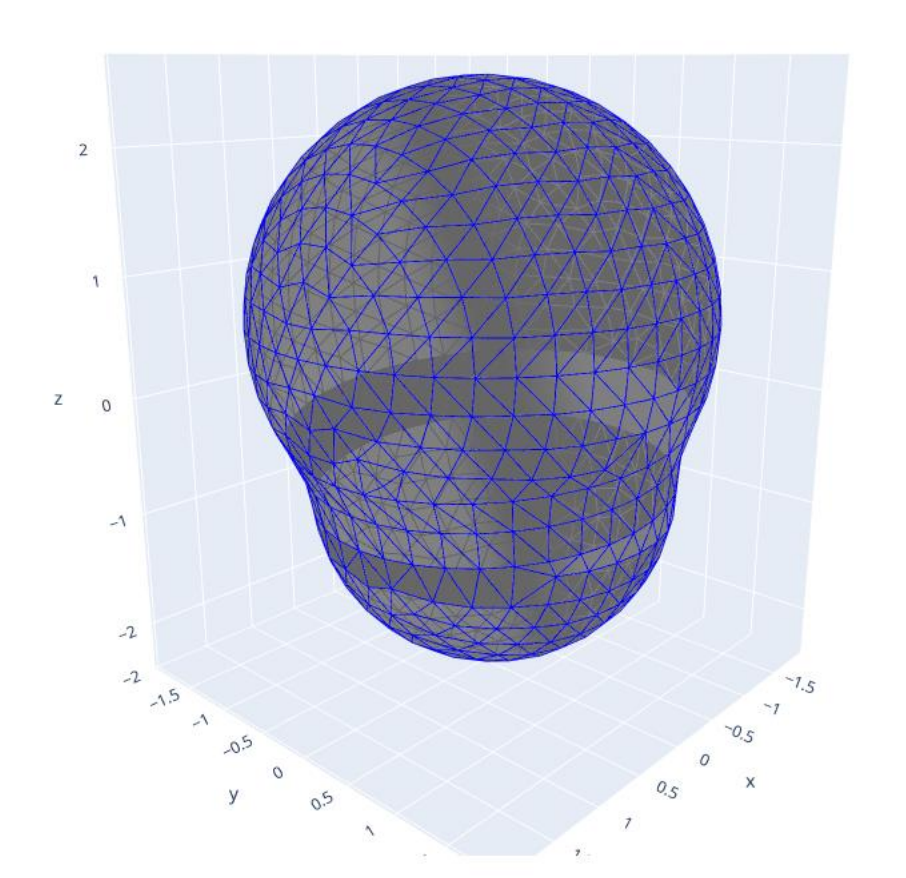


Loss History of NN2, Iterations: 10000, Loss: 7.787e-05
Loss_XN
Loss_NN
Loss_R
Loss_D
Loss_K
Loss_Iu
Loss_Id
Loss_E
$\mathcal{L}: Losses$
$n: iterations$

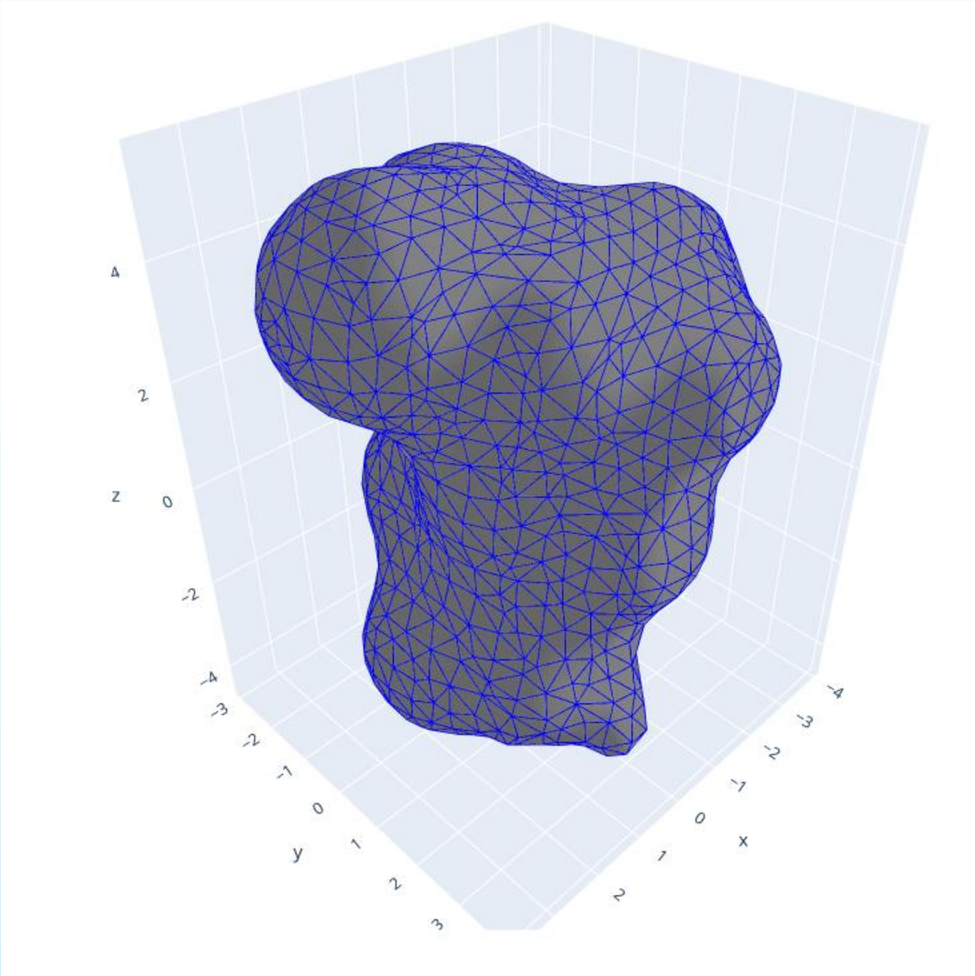


Solution G_{solv} of PDE, Iterations: 10000, G_solv: -33.43 kcal/kmol
G_solv
G_{solv}
$n: iterations$

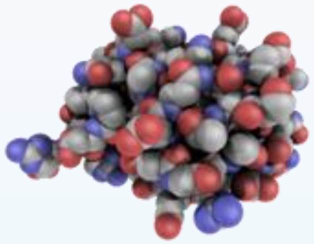
Methanol



Arginine



Conclusions



- **Fourier features** and **weights balancing** algorithm are **needed** for good results.
- Point data loss term is **required** for quick convergence.
- Experimental loss term (ϕ_{ENS}) **improve**s convergence
- Gauss Law loss term makes the solution to diverge. (Integral loss term?).
- Full batch approach works fine to this problem. Samples or multiple batches can be tested.
- Bigger molecules increase complexity and reduces the precision of the XPINN solver.
- More tests are needed. Will be useful for “big” molecules?

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XPINN Solver for 3D Poisson-Boltzmann Equation

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