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A Solution of a $3d$ Cartesian Poisson-Boltzmann Equation

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Abstract

We solve the 3d-Cartesian Poisson-Boltzmann equation (PBEq) for a 1 : 1 electric charge configuration, using the tanh, Ricatti functions and Jacobi elliptic solitary wave methods. Also, we apply a deep learning algorithm, specifically, physics-informed neural networks (PINNs), which is implemented in a Python library known as DeepXDE, finding good agreement between the analytical and the PINNs results.

Keywords: 3d Poisson-Boltzmann equation, Tanh method, Ricatti functions, Jacobi elliptic functions, Deep Learning, DeepXDE

1 Introduction

Over the years Poisson Boltzmann equation has remained as a great challenge for the world of engineering and science [1], leaving its practical use in the field of computational methods [2]. On the other hand, traveling wave solutions are a very useful mathematical methods in order to find solutions to nonlinear partial differential equations (NPDEs), [3]-[6]. Otherwise, Physics informed neural networks (PINN) are a particular class of neural networks (NN) that simulates and predicts solutions to problems where the underlying mathematical physics laws, differential equations, are known [7]-[9]. In this work, we obtain and contrast analytical solutions with the solution provided by PINNs, using the software DeepXDE [9].

2 $3d$ Cartesian Poisson-Boltzmann equation

The $3d$ Cartesian Poisson-Boltzmann equation is:

$$\frac{\partial^2\phi}{dx^2} + \frac{\partial^2\phi}{dy^2} + \frac{\partial^2\phi}{dz^2} = -\kappa^2(e^{(-\phi)} - e^{(\phi)}) \tag{1}$$

Where κ^{-1} is the Debye's screening length [1]. Also, we use the next coordinate transformation and its derivatives, as:

$$\xi + \xi_0 = x + y + z, \quad \frac{d^2}{d\xi^2} = \frac{d^2}{dx^2} = \frac{d^2}{dy^2} = \frac{d^2}{dz^2} \tag{2}$$

Therefore, eq. (1) is:

$$3\frac{d^2}{d\xi^2}\phi = \kappa^2(-e^{(-\phi)} + e^{(\phi)}) \tag{3}$$

Now, we define the variables:

$$v = v_0 e^{\phi}, \;\; v^{-1} = v_0^{-1} e^{-\phi} \tag{4}$$

So, the first and second derivatives in eq. (3), are:

$$\frac{d\phi}{d\xi} = \frac{1}{v}\frac{dv}{d\xi}, \;\; \frac{d^2\phi}{d\xi^2} = -\frac{1}{v^2}(\frac{dv}{d\xi})^2 + \frac{1}{v}\frac{d^2v}{d\xi^2} \tag{5}$$

And replacing in eqs. (3)

$$-\frac{1}{v^2}(\frac{dv}{d\xi})^2 + \frac{1}{v}\frac{d^2v}{d\xi^2} = \frac{\kappa^2}{3}(-\frac{v_0}{v} + \frac{v}{v_0}) \tag{6}$$

So

$$-v_0(\frac{dv}{du})^2 + v_0 v\frac{d^2v}{du^2} + \frac{\kappa^2}{3}v_0^2 v - \frac{\kappa^2}{3}v^3 = 0 \tag{7}$$

Now, we introduce a new independent variable [3]:

$$Y = \tanh(\mu u) \tag{8}$$

Then, the derivatives of u, are:

$$\frac{d}{du} = \mu(1 - Y^2)\frac{d}{dY}, \;\; \frac{d^2}{du^2} = -2Y\mu^2(1 - Y^2)\frac{d}{dY} + \mu^2(1 - Y^2)^2\frac{d^2}{dY^2} \tag{9}$$

The solutions are postulated as [3]:

$$v = \sum_{i=1}^{m} a_i Y^i \tag{10}$$

Then replacing

$$-2v_0 v\mu^2 Y(1-Y^2)\frac{dv}{dY} + v_0 v\mu^2(1-Y^2)^2\frac{d^2v}{dY^2} - v_0\mu^2(1-Y^2)^2(\frac{dv}{dY})^2 \tag{11}$$
$$+\frac{\kappa^2}{3}v_0^2 v - \frac{\kappa^2}{3}v^3 = 0$$

Now, we balance the highest-order linear derivative with the highest order nonlinear terms in eq. (18) and eq. (19). Then, $vY^4\frac{d^2v}{dY^2} \to v^3 \to m = 2$. So, replacing in eq. (17)

$$v = a_0 + a_1 Y + a_2 Y^2 \tag{12}$$

Replacing in eqs. (18)), we get a set of equations, order by order in Y^i. Doing some algebra, we get:

$$f_1 \to (a_0 = 0, a_1 = 0, a_2 = v_0, \mu = -\kappa\frac{1}{\sqrt{6}v_0}) \tag{13}$$

$$f_2 \to (a_0 = 0, a_1 = 0, a_2 = -v_0, \mu = -i\kappa\frac{1}{\sqrt{6}v_0}) \tag{14}$$

$$f_3 \to (a_0 = 0, a_1 = 0, a_2 = -v_0, \mu = i\kappa\frac{1}{\sqrt{6}v_0}) \tag{15}$$

$$f_4 \to (a_0 = 0, a_1 = 0, a_2 = v_0, \mu = \kappa\frac{1}{\sqrt{6}v_0}) \tag{16}$$

Then, we get four families of solutions.

3 Solitary wave method 2, Solutions Riccati equation

We use the method in [4], to get solutions for eqs. (6). So:

	A_1	C_1	F
1	1/2	-1/2	$coth(\xi) \pm cosh(\xi)$, $tanh(\xi) \pm isech(\xi)$
2	1/2	1/2	$sec(\xi) \pm itan(\xi)$
3	-1/2	- 1/2	$csc(\xi) \pm icot(\xi)$
4	1	- 1	$tanh(\xi)$, $coth(\xi)$
5	1	1	$tan(\xi)$
6	-1	-1	$cot(\xi)$

Table 1: Solutions for eqs. (7), [4] .

$$v = \sum_{i=1}^{n} a_i F^i \tag{17}$$

where F solves, table (1), the Riccati equation, i.e.

$$F^{'} = (C_1 F^2 + A_1), \quad F^{''} = 2C_1 F(C_1 F^2 + A_1) \tag{18}$$

here A_1 and C_1 are constants, table (1). Replacing in eqs. (6), and balancing nonlinear terms, we have $n = 2$. Then, eq. (25) is, $v = (a_0 + a_1 F + a_2 F^2)$. Therefore, the derivatives are:

$$\begin{aligned} v^{'} = (a_1 + 2a_2 F)F^{'} = (a_1 + 2a_2 F)(C_1 F^2 + A_1), \;\; v^{''} = ((2a_2 F^{'})F^{'} \\ +(a_1 + 2a_2 F)F^{''}) = (2a_2(C_1 F^2 + A_1)^2 + (a_1 + 2a_2 F)2C_1 F(C_1 F^2 + A_1)) \end{aligned} \tag{19}$$

Replacing in eq. (6), we obtain a group of equations, order by order in F^i. Doing algebra, we get:

$$g_1 \leftarrow (a_0 = 0, a_1 = 0, a_2 = \frac{C_1 v_0}{A_1}, \kappa = -\sqrt{6A_1C_1}) \tag{20}$$

$$g_2 \leftarrow (a_0 = 0, a_1 = 0, a_2 = -\frac{C_1 v_0}{A_1}, \kappa = -i\sqrt{6A_1C_1}) \tag{21}$$

$$g_3 \leftarrow (a_0 = 0, a_1 = 0, a_2 = -\frac{C_1 v_0}{A_1}, \kappa = i\sqrt{6A_1C_1}) \tag{22}$$

$$g_4 \leftarrow (a_0 = 0, a_1 = 0, a_2 = \frac{C_1 v_0}{A_1}, \kappa = \sqrt{6A_1C_1}) \tag{23}$$

Then, we get twenty four families of solutions, g_i, using Ricatti method [4].

	ϵ	a	b	c	G
1	-1	$-m^2$	1	1	$sn(\xi)$
2	-1	m^2	$1-m^2$	1	$cn(\xi)$
3	-1	1	m^2-1	1	$dn(\xi)$
4	-1	$-m^2$	1	1	$cd(\xi)$
5	m^2-1	m^2	1	1	$sd(\xi)$
6	$1-m^2$	1	-1	1	$nd(\xi)$
7	1	1	$-m^2$	-1	$dc(\xi)$
8	1	$1-m^2$	m^2	-1	$nc(\xi)$
9	1	$1-m^2$	1	1	$sc(\xi)$
10	1	1	$-m^2$	-1	$ns(\xi)$
11	1	1	m^2-1	m^2	$ds(\xi)$
12	1	1	$1-m^2$	1	$cs(\xi)$

Table 2: The Solutions for eq. (24), [5] .

4 Solitary wave method 3, Jacobi solutions

We start with the solutions, table (2), given by the next differential equation:

$$(G^{'})^2 = (c + \epsilon G^2)(aG^2 + b) \tag{24}$$

Also, they satisfy the next relations:

$$\begin{aligned} & sn(\xi,k)^2 + cn(\xi,k)^2 = k^2 sn(\xi,k)^2 + dn(\xi,k)^2 = 1 \\ & 1 + cs(\xi,k)^2 = k^2 + ds(\xi,k)^2 = ns(\xi,k)^2 \\ & (1-k^2)sd(\xi,k)^2 + 1 = dc(\xi,k)^2 = (1-k^2)nc(\xi,k)^2 + k^2 \\ & k^2(1-k^2)sd(\xi,k)^2 = k^2(cd(\xi,k)^2 - 1) = (1-k^2)(1 - nd(\xi,k)^2) \end{aligned} \tag{25}$$

and $k^{'} = sqrt(1-k^2)$

$$\begin{aligned} & sn(i\xi,k) = (i)sn(\xi,k^{'}), \quad dc(i\xi,k) = dn(\xi,k^{'}) \\ & cn(i\xi,k) = nc(\xi,k^{'}), \quad nc(i\xi,k) = cn(\xi,k^{'}) \\ & dn(i\xi,k) = dc(\xi,k^{'}), \quad sc(i\xi,k) = (i)sn(\xi,k^{'}) \\ & cd(i\xi,k) = nd(\xi,k^{'}), \quad ns(i\xi,k) = (-i)cs(\xi,k^{'}) \\ & sd(i\xi,k) = (i)nd(\xi,k^{'}), \quad ds(i\xi,k) = (-i)ds(\xi,k^{'}) \\ & nd(i\xi,k) = cd(\xi,k^{'}), \quad cs(i\xi,k) = (-i)ns(\xi,k^{'}) \end{aligned} \tag{26}$$

and the second derivative is:

$$G'' = 2a\epsilon^2 G^3 + (ac+b)\epsilon G \tag{27}$$

Where a, b, c and ϵ are given in table (2). We use the method in [6], to get solutions for eqs. (6).

$$v = \sum_{i=1}^{n} a_i G^i \tag{28}$$

Replacing eqs. (24) and (27) in eq. (6), and balancing nonlinear terms, we have $n = 2$. Therefore, the solution is:

$$v = (a_0 + a_1 G + a_2 G^2) \tag{29}$$

Then, we obtain a group of equations, order by order in G^i. And doing some algebra, we get:

$$\begin{aligned} g_1 \leftarrow (a_0 &= -\frac{\sqrt{-1+2\epsilon}v_0}{\sqrt{6}\sqrt{\epsilon}}, a_1 = \frac{1}{2\epsilon}, a_2 = 0, \\ a &= -\frac{\kappa^2}{8\sqrt{6}\epsilon^{9/2}\sqrt{-1+2\epsilon}v_0^3}, b = \frac{\sqrt{-1+2\epsilon}\kappa^2}{12\sqrt{6}\epsilon^{7/2}v_0}, \\ c &= -\frac{2}{3}\epsilon^2(1+4\epsilon)v_0^2) \end{aligned} \tag{30}$$

$$\begin{aligned} g_2 \leftarrow (a_0 &= -\frac{\sqrt{-1+2\epsilon}v_0}{\sqrt{6}\sqrt{\epsilon}}, a_1 = \frac{1}{2\epsilon}, a_2 = 0, \\ a &= -\frac{\kappa^2}{8\sqrt{6}\epsilon^{9/2}\sqrt{-1+2\epsilon}v_0^3}, b = \frac{(1+4\epsilon)\kappa^2}{12\sqrt{6}\epsilon^{7/2}\sqrt{-1+2\epsilon}v_0}, \\ c &= -\frac{2}{3}\left(-\epsilon^2 v_0^2 + 2\epsilon^3 v_0^2\right)) \end{aligned} \tag{31}$$

$$\begin{aligned} g_3 \leftarrow (a_0 &= \frac{\sqrt{-1+2\epsilon}v_0}{\sqrt{6}\sqrt{\epsilon}}, a_1 = \frac{1}{2\epsilon}, a_2 = 0, \\ a &= \frac{\kappa^2}{8\sqrt{6}\epsilon^{9/2}\sqrt{-1+2\epsilon}v_0^3}, b = -\frac{\sqrt{-1+2\epsilon}\kappa^2}{12\sqrt{6}\epsilon^{7/2}v_0}, \\ c &= -\frac{2}{3}\epsilon^2(1+4\epsilon)v_0^2) \end{aligned} \tag{32}$$

NN depth	*NN width*	*Optimizer*	*Learning rate*	*#Iterations*
3	$30, 60, 90$	*Adam*	0.001	20000

Table 3: Hyperparameters [**?**].

width	*train loss*	*test loss*	*test metric*
20	$4.35e-06$	$5.57e-04$	$3.59e-02$
60	$3.46e-06$	$5.30e-04$	$3.72e-02$
100	$1.30e-04$	$1.70e-04$	$9.49e-02$

Table 4: Models trained with a changing width $(20, 60, 100)$ for 20000 steps. Also, the train and test loss and test metric values of the models are shown.

$$
\begin{aligned}
&g_4 \leftarrow (a_0 = \frac{\sqrt{-1+2\epsilon}v_0}{\sqrt{6}\sqrt{\epsilon}}, a_1 = \frac{1}{2\epsilon}, a_2 = 0, \\
&a = \frac{\kappa^2}{8\sqrt{6}\epsilon^{9/2}\sqrt{-1+2\epsilon}v_0^3}, b = -\frac{(1+4\epsilon)\kappa^2}{12\sqrt{6}\epsilon^{7/2}\sqrt{-1+2\epsilon}v_0}, \\
&c = -\frac{2}{3}\left(-\epsilon^2 v_0^2 + 2\epsilon^3 v_0^2\right))
\end{aligned}
\tag{33}
$$

Then, we get forty eight families of solutions, g_i, using Jacobi solutions [6].

5 A solution using DeepXDE

Then, we will solve an ODE eq. (2) using the library given in [9]. We define $\mu = 1.6 * \sqrt{6}$ in the set of solutions given by eq. (11), and with initial conditions $\phi(0) = -0.16, \phi'(0) = 1.26$. For a domain $\xi \in [0, 5.1]$. The exact solution is $\phi(\xi) = \ln\left\{\frac{\tanh^2(\mu(\xi+0.41))}{v_0}\right\}$. We use the tanh as the activation function, and the hyperparameters are given in table (3).

We utilize a fully connected neural network of depth 4, with 3 hidden layers, and variable width of $(20, 60, 100)$. Also, the number of training residual points are 16 an are sampled inside the domain, and 2 is the number of training points used on the boundary. At last, we define 500 residual points for probing the ODE residual.

The results applying PINN algorithm [9] for solving eq. (33) are presented in figures (1-4). The solid black line is the exact solution, fig. (1), and the dashed red line is the predicted solution from PINN, join with the black dotted trained points, finding good agreement. Additionally, the results for widths $(20, 60, 100)$, are presented in figures (2-4), the difference between train and test loss remain small and constant, for all the three widths.

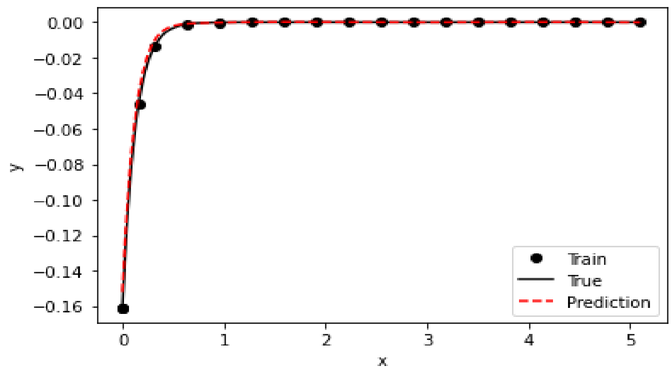

Figure 1: Analytical solution, predicted results and trained points.

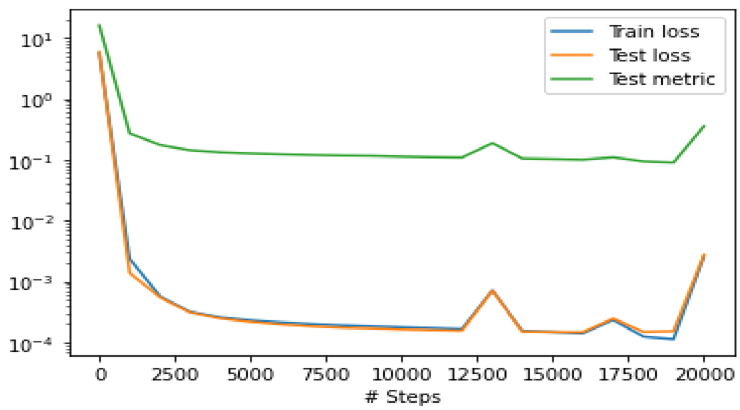

Figure 2: width = 20.

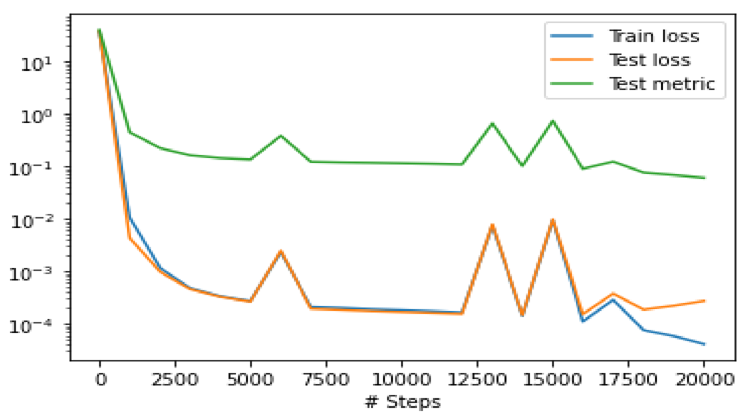

Figure 3: width = 60.

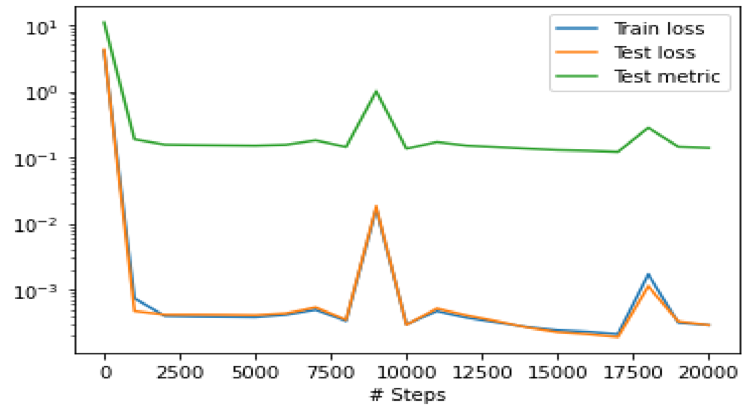

Figure 4: width = 100.

6 Conclusions

We solve a 3d Cartesian Poisson-Boltzmann equation applying several solitary wave methods. So, using tanh method we find four families of solutions. In addition, using the Ricatti functions, we get twenty four families of solutions. likewise, utilizing Jacobi elliptic functions, we obtain forty eight families of solutions. At last, we apply PINNs using DeepXDE library [9], finding good agreement between analytical solution and the deep learning outcomes. The analytical solutions are:

$$\phi = \ln\left(\frac{(a_2 \tanh^2(\mu u))}{v_0}\right), \ \phi = \ln\left(\frac{(a_2 F^2(u))}{v_0}\right), \ \phi = \ln\left(\frac{(a_0 + a_1 G(u))}{v_0}\right) \quad (34)$$

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