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Physics-Informed Graph Neural Network for Circuit Compact Model Development

Xujiao Gao
Electrical Models & Simulation
Sandia National Laboratories
Albuquerque, USA
xngao@sandia.gov

Andy Huang
Electrical Models & Simulation
Sandia National Laboratories
Albuquerque, USA
ahuang@sandia.gov

Nathaniel Trask
Computational Mathematics
Sandia National Laboratories
Albuquerque, USA
natrask@sandia.gov

Shahed Reza
Component & Systems Analysis
Sandia National Laboratories
Albuquerque, USA
sreza@sandia.gov

***Abstract*—We present a Physics-Informed Graph Neural Network (pigNN) methodology for rapid and automated compact model development. It brings together the inherent strengths of data-driven machine learning, high-fidelity physics in TCAD simulations, and knowledge contained in existing compact models. In this work, we focus on developing a neural network (NN) based compact model for a non-ideal PN diode that represents one nonlinear edge in a pigNN graph. This model accurately captures the smooth transition between the exponential and quasi-linear response regions. By learning voltage dependent non-ideality factor using NN and employing an inverse response function in the NN loss function, the model also accurately captures the voltage dependent recombination effect. This NN compact model serves as basis model for a PN diode that can be a single device or represent an isolated diode in a complex device determined by topological data analysis (TDA) methods. The pigNN methodology is also applicable to derive reduced order models in other engineering areas.**

Keywords—physics informed graph neural network (pigNN), compact model development, topological data analysis (TDA), TCAD, non-ideality factor, Shockley-Read-Hall

I. Introduction

To rapidly reduce the often multi-year cycle of reliable circuit compact model development (CMD), data-driven machine learning (ML) methods have recently been employed to derive compact models [1-3] and even optimize design at the circuit level [4-5]. However, as clearly recognized in [6], compact models generated from data-driven ML can lead to unphysical results due to the nature of a physics-agnostic method. To address this issue, researchers have tried to analytically formulate the most significant physics for a given device as constraints in the ML training [6]. The obvious drawback with this remedy is that only a few components of the entire complex device physics are considered, so the resulting compact model (CM) is still not predictive outside the training data range. Most recently, data-driven NN models with ties to PDEs are being investigated [7] for CMD, and inspired the ML training used in this work. However, their models rely on device terminal response data and ignore the internal physical information offered by technology aided computer design (TCAD) simulation. To incorporate and facilitate TCAD in CMD, we propose a Physics-Informed Graph Neural Network (pigNN) methodology for rapid and automated CMD, which brings together the inherent strengths of data-driven ML, high-fidelity physics in TCAD simulation, and knowledge contained in existing compact models.

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II. Methodology

The motivating principle grounding our methodology lies in a fundamental shift in the order of compact model construction. Traditionally, a circuit CM is obtained by piecing together individual geometry-independent electronic components, informed by adjacent and correlated physical phenomena within the device. Our proposed pigNN methodology reverses the order of CM assembly: first, we use TCAD device simulation results to identify the graph topology physically intrinsic to a given device accounting for important physical effects; then, we deduce the circuit components required to populate the graph in order to form the circuit CM.

As depicted in Fig. 1, our pigNN workflow contains four stages. First, during the Physics Priming (PP) stage, loosely calibrated TCAD device models are used to simulate a given device throughout its operating regime. We use Sandia's open-source TCAD Charon [8] code which allows us to have full access to physical quantities. Second, physically significant regions are identified (RR stage). From the concert of physical fields, we determine physically important regions as they evolve through a sweep of bias/time conditions. ML classification and Topological Data Analysis (TDA) for processing the fields are the primary tools in this stage. Third, we process the data from stage RR using TDA and graph cut techniques to seed a ML process to determine the intrinsic device topology (TT stage). Finally, electronic components are selected to functionally represent the physical interactions along the edges of a device topology (II stage). In this stage, established compact models (ECM) will be utilized to guide the interaction identification; Sandia's Xyce simulator [9] is used for circuit simulation, allowing us to streamline pigNN-based compact models directly into Xyce. Stages RR, TT, and II are trained and adapted using available experimental data until a robust physics-informed CM is achieved.

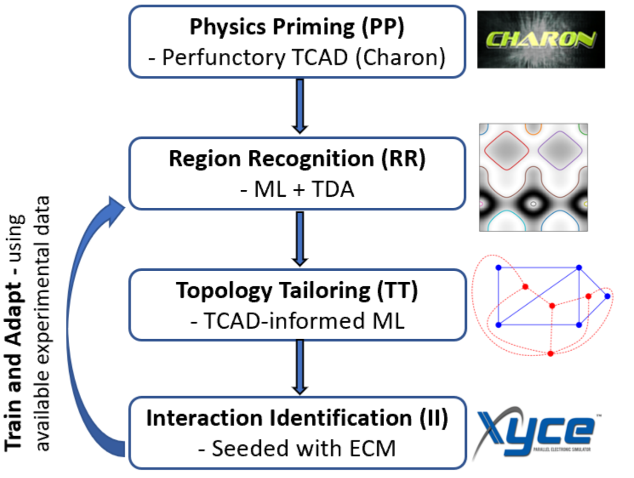

Fig. 1. Workflow of the pigNN-CMD methodology. The second and third graphs in the right column are taken from Wikipedia for illustration purpose only.

III. Application Example

Details of the pigNN methodology are described in [10] where pigNN is demonstrated on a 2D resistor network and a nonlinear non-CMD problem [10]. For the 2D resistor problem, a spectral partitioning scheme (a TDA method) [10] was used to determine important physical regions based on TCAD solutions, which map to a linear resistor network. The TensorFlow based NN was used to achieve parameter-free learning by enforcing Kirchhoff's current law at each node via partial different equation (PDE) constrained optimization.

To move beyond linear elements, the most important non-linear device for CMD is a PN diode. Multiple PN diodes are widely used in compact models of semiconductor devices. Before we can model multiple PN diodes or mixed electronic components in a graph using pigNN, we need to first build an accurate compact model for a non-ideal diode that represents one edge in a pigNN graph. In this work, we focus on developing NN based compact model for a non-ideal PN diode under forward bias. A single PN diode represents an isolated PN junction determined by TDA based on spatial physical quantities such as electric potential and/or space charge profiles in a real device. The obtained NN compact model will serve as PN diode model basis in a complex device.

We started by simulating an arbitrarily selected silicon 1D PN diode in Charon. It is 0.5-µm long in both P and N sides and has a symmetric, uniform doping of 10^{16} cm^{-3}. Our baseline TCAD simulation used the most basic physical models such as constant mobility and absence of recombination/generation processes. For this baseline case, the simulated results from Charon are shown as solid lines in Fig. 2. It is well-known that the current-voltage (I-V) curve for a non-ideal PN diode shows an exponential region and a quasi-linear region. TCAD simulation naturally captures the smooth transition from exponential to quasi-linear response. However, popular diode compact models [11] cannot model a smooth transition switching between the two regimes. Even in the quasi-linear regime, the diode conductance is not constant, but varies nonlinearly with voltage as seen in the inset of Fig. 2. Bandwell and Jayakumar [12] proposed using the Lambert W-function to smoothly interpolate the exponential and the quasi-linear regions without a switch. However, the model does not incorporate a voltage dependent non-ideality factor, which can account for the voltage dependent recombination process governed by the carrier transport drift diffusion continuity equations.

To develop a compact model that captures the diode's smooth I-V response determined by TCAD physics, we propose the following CM for the edge current in a pigNN graph:

$$I_D = [1 - w(V_D)]I_0\left(e^{\frac{qV_D}{\eta k_B T}} - 1.0\right) + w(V_D)(V_D - V_{tr})G_0$$
$$+ w(V_D)(V_D - V_{tr})G_{NN}(V_D). \quad (1)$$

Here $w(V_D)$ is a voltage dependent weighting function, i.e.,

$$w(V_D) = 0.5[\tanh(10^5(V_D - V_{tr})) + 1.0], \quad (2)$$

which is a step-like but smooth function between 0 and 1 with the transition occurring at V_{tr}. The factor of 10^5 controls how steep the transition occurs, which is a heuristic value at this point. We will explore initializing the factor from physical fields contained in TCAD results. $G_{NN}(V_D)$ is a NN component to model the voltage dependent conductance in the quasi-linear regime. Other variables learned by NN are I_0, η, V_{tr}, and G_0. We used the TensorFlow library [13] to train the neural network and model parameters. Equation (1) can be interpreted as a diode, a constant conductance, and a voltage dependent conductance in parallel. However, the diode is turned on when $V_D < V_{tr}$ and the conductance branches are turned on when $V_D \geq V_{tr}$. The transition is determined by the smooth function in (2). To compare the NN learned conductance with Charon simulation result, we rewrite (1) as

$$I_D = [1 - w(V_D)]I_0\left(e^{\frac{qV_D}{\eta k_B T}} - 1.0\right) + V_D G_D(V_D), \quad (3)$$

where $G_D(V_D)$ is the diode conductance in the quasi-linear region and given by

$$G_D(V_D) = w(V_D)\left(1 - \frac{V_{tr}}{V_D}\right)G_0 + w(V_D)\left(1 - \frac{V_{tr}}{V_D}\right)G_{NN}. \quad (4)$$

Using initial values obtained from simulated I-V results for the learning variables, we achieved excellent agreement between the NN based CM (dots in Fig. 2) and TCAD results (solid lines in Fig. 2) for our baseline diode.

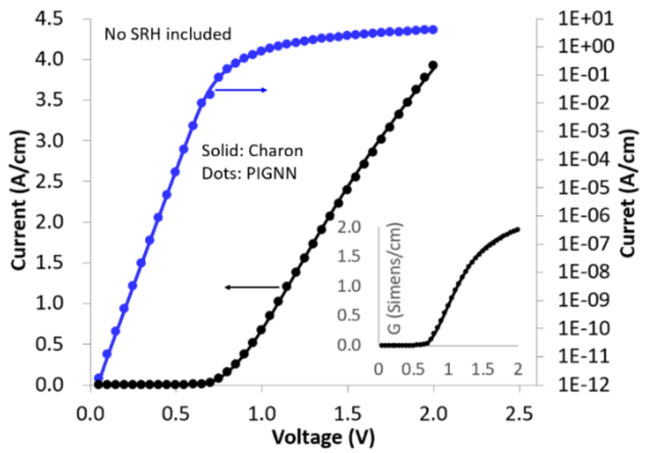

Fig. 2. Diode current-voltage comparison between Charon (solid lines) and pigNN learned results (dots) in both linear (left axis) and log (right axis) scales for the case of no SRH. Inset shows the diode conductance, $G_D(V_D)$, vs. voltage comparison between Charon (solid) and pigNN (dots).

It is well-known that the non-ideality factor η in (1) may model the Shockley-Read-Hall (SRH) recombination effect in the low forward bias region. As a next step, we enabled the SRH recombination in our Charon simulation of the diode with four different carrier lifetimes. Charon results are shown as solid lines in Fig. 3. Using the compact model in (1), the NN learned I-V curves (dots in Fig. 3) match Charon results quite well except in the exponential region. The learned diode conductance, $G_D(V_D)$, in the quasi-linear region, are in excellent agreement with Charon simulated conductance as shown in Fig. 4. Note the diode conductance has a strong non-linear voltage dependence.

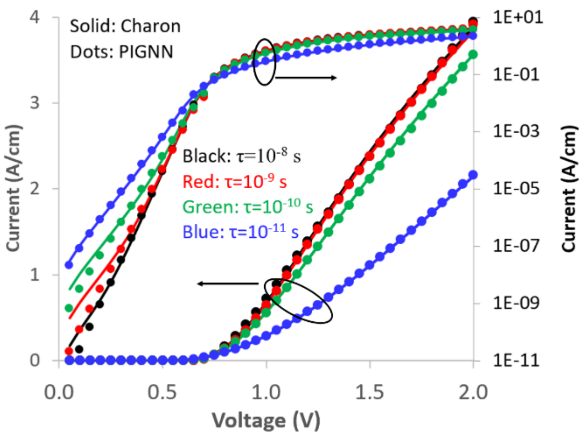

Fig. 3. Diode current-voltage comparison between Charon (solid lines) and pigNN results (dots) in both linear (left axis) and log (right axis) scales for TCAD simulations including SRH with 4 different carrier lifetimes.

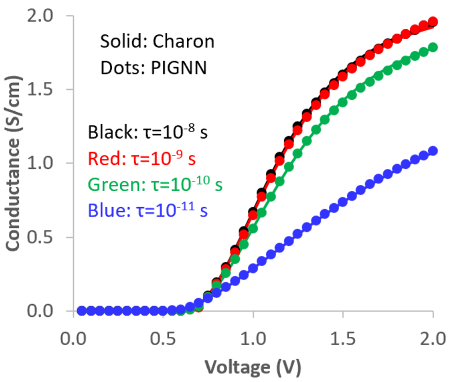

Fig. 4. Diode conductance, $G_D(V_D)$, vs. voltage comparison between Charon (solid) and pigNN (dots) for the same simulations as in Fig. 3.

We see in Fig. 3 that the NN learned I-V responses did not accurately reproduce the Charon results in the exponential region. This is because our NN compact model above used a voltage independent non-ideality factor, η, for a given carrier lifetime, while the Charon simulation naturally captures the voltage dependent SRH recombination effect. The pigNN learned variables for the results shown in Figs. 3-4 are listed in Table I. Clearly, the leakage current (I_0) and the non-ideality factor (η) both increase with decreasing lifetime (τ), i.e., increased SRH recombination, as expected, since they are both directly associated with recombination processes. The transition voltage (V_{tr}) is somewhat related to the built-in potential of a diode, so its value does not change much until at a very short lifetime. The constant conductance (G_0) is more a fitting parameter than related to any physical quantity, while the important conductance quantity is the diode conductance, $G_D(V_D)$, defined in (4).

TABLE I. PIGNN LEARNED VARIABLES FOR RESULTS IN FIG. 3

τ (s)	I_0 (A/cm)	η	V_{tr}	G_0
No SRH	1.71×10^{-13}	1.0	0.68	2.82
10^{-8}	1.35×10^{-12}	1.13	0.71	1.79
10^{-9}	5.14×10^{-12}	1.21	0.68	2.30
10^{-10}	2.37×10^{-10}	1.46	0.67	1.89
10^{-11}	1.02×10^{-8}	1.75	0.57	0.37

It is clear that a voltage independent non-ideality factor in a diode compact model cannot correctly capture the SRH recombination effect. To include the recombination effect in our compact model (1), we apply NN to learn the voltage dependent non-ideality factor. Since we know $\eta = 1$ for the case of no recombination, we rewrite $\eta(V_D) = 1 + \eta_{NN}(V_D)$ with $\eta_{NN}(V_D)$ being the NN-learned factor accounting for the recombination effect. With two NN-learned components in the model (1), we find the choice of the NN loss function becomes very important. When η is voltage independent, we can achieve decent results shown in Figs. 3-4 by defining the NN loss function as $\mathcal{L} = (I_{NN} - I_t)^2/I_t^2$. Here I_t is the target current obtained from either experiment or TCAD simulation, and I_{NN} is the NN learned current. When using NN to learn $\eta_{NN}(V_D)$, we find this simple loss function is insufficient due to the twelve order of magnitude difference in the current response. A good loss function seems to be a mixture of a logarithmic function (for the exponential I-V region) and a linear function (for the quasi-linear region). However, it is difficult heuristically figuring out a proper weighting of the two functions. To address this challenge, we propose to incorporate an approximate inverse (i.e., voltage-current) function of the target I-V response in the NN loss function. Specifically, given a I-V response, we can apply a regression method to obtain a function that approximates the voltage as a function of the current. We stress that an approximation is sufficient since it is only used in the loss function. Fig. 5 shows a comparison between the approximate V-I curve (red line) and the Charon result for the case of $\tau = 10^{-9}$ s. There exist many possible functions to approximate a diode V-I response. We somewhat arbitrarily chose this form: $\upsilon(I) = (aI)^b \times \tanh(dI - e) + fI$, where υ and I represent voltage and current, respectively, *a, b, d, e, f* are parameters that can be determined using a regression method. We used the Python sci.optimize module to obtain these parameters. Then we define the loss function as $\mathcal{L} = [\upsilon(I_{NN}) - \upsilon(I_t)]^2/[\upsilon(I_t)]^2$. The $\upsilon(I)$ function maps the logarithmically separated current range (twelve orders of magnitude) to a linearly separated voltage range, which allows us to effectively minimize the error between learned and target currents.

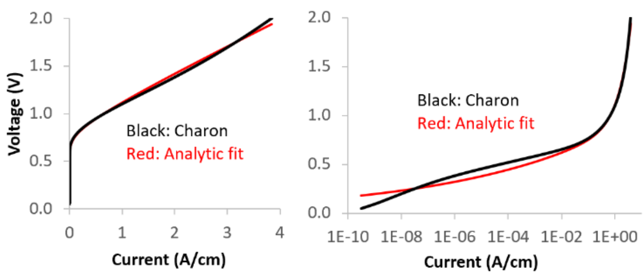

Fig. 5. Approximate voltage-current function (red line) of the Charon result for the case of $\tau = 10^{-9}$ seconds (black line) on the linear current scale (left panel) and the log scale (right panel).

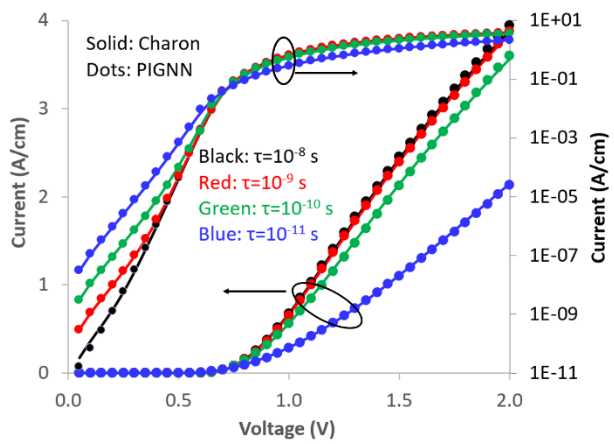

Fig. 6. Diode current-voltage comparison between Charon (solid lines) and pigNN results (dots) obtained using voltage-dependent non-ideality factors in both linear (left axis) and log (right axis) scales for TCAD simulations including SRH with four different carrier lifetimes.

Using the compact model in (1) with voltage dependent NN-learned non-ideality factor $\eta(V_D)$ and the proposed loss function, we achieve excellent agreement between pigNN and Charon results as shown in Fig. 6 in both the exponential and linear regions for the four different carrier lifetimes. The NN-learned $\eta(V_D)$ for the pigNN results in Fig. 6 are plotted in Fig. 7 as a function of voltage for different lifetimes. Except for the largest lifetime of 10^{-8} seconds, the non-ideality factors for other three cases start around 2 at the lowest voltage point and decrease with increasing voltages. We know from semiconductor physics that a pure recombination current yields a non-ideality of 2. Therefore, our NN-learned non-ideality factor is consistent with the physics that the SRH recombination dominates the current at low voltages and its effect decreases with increasing voltages. As the forward voltage increases, the PN junction barrier is reduced, so the diffusion current becomes more dominant, until the drift current takes over in the quasi-linear current-voltage regime. For the case of 10^{-8}-second lifetime, the non-ideality factor shows an opposite trend in the low voltages. This is more numerical than physical since the recombination effect is very small at this lifetime. Note that the non-ideality factor values have no significance for voltages above the transition voltages V_{tr}, which are listed in Table II for the pigNN results shown in Fig. 6. This is because our compact model in (1) contains a weighting function that smoothly masks out the diode response for voltages above V_{tr}.

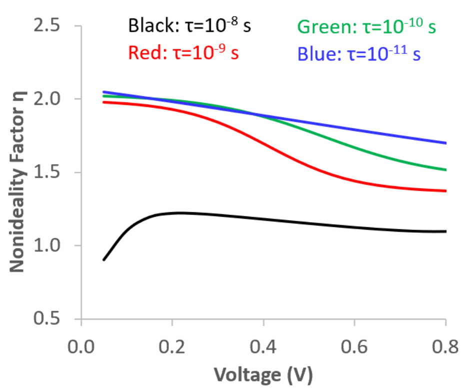

Fig. 7. NN learned non-ideality factor $\eta(V_D)$ as a function of voltage for the pigNN results shown in Fig. 6.

TABLE II. PIGNN LEARNED PARAMETERS FOR RESULTS IN FIG. 6

τ (s)	I_0 (A/cm)	V_{tr} (V)	G_0 (S/cm)
10^{-8}	2.22×10^{-12}	0.62	2.50
10^{-9}	1.85×10^{-10}	0.63	1.63
10^{-10}	1.87×10^{-9}	0.57	1.46
10^{-11}	1.96×10^{-8}	0.52	0.83

IV. CONCLUSIONS

We have presented a Physics-Informed Graph Neural Network (pigNN) methodology for rapid and automated compact model development, which brings together the inherent strengths of data-driven ML, high-fidelity physics in TCAD simulation, and knowledge contained in existing compact models. Using data-driven neural network, we have developed an accurate compact model of a non-ideal PN diode that represents one nonlinear edge in a pigNN graph. A PN diode can be a single device or one isolated diode in a complex device determined by TDA methods. The NN compact model accurately captures the smooth transition between the exponential and quasi-linear response regions and the voltage-dependent recombination effect in a non-ideal PN diode under forward bias. We are applying the full pigNN methodology which enforces Kirchhoff's current law at each node in a pigNN graph to develop compact models for bipolar transistors. The methodology is also being explored to derive reduced order models in other engineering areas such as mechanics and electromagnetics.

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