

# Multi-order Differential Neural Network for TCAD Simulation of<br>
the Semiconductor Devices<br>
Ties Cai\*
AnAoxue Huang\*
Tieng Xiong\*
Tieng Xiong\*
1575803685@qq.com
1333227546@qq.com
27988214@qq.com
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Andoxue Huang\***<br>
Andoxue Huang\*<br>
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Xiangshui Miao\*<br>
Ningsheng Wang\*<sup>†</sup><br>
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Ningsheng Wang\*<sup>†</sup><br>
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Zifei Cai\* AnAoxue Huang\* Yifer<br>
803685@qq.com 1353227546@qq.com 327988<br>
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105136@qq.com miaoxs@hust.edu.cn xs **i-order Differential Neural Network for TCAD Sim**<br> **the Semiconductor Devices**<br>  $\text{Zifei Cai*} \qquad \text{An} \text{Aoxue Huang*} \qquad \text{Yifeng} \qquad \text{Yifeng} \qquad \text{S803685@qq.com}$ <br>  $\text{Dejiang Mut*} \qquad \text{Xiangshui Miao*} \qquad \text{Xingshei} \qquad \text{Xingshei} \qquad \text{M105136@qq.com}$ <br>  $\text{CFT}$ EUTAL Network for TCAD Simulation of<br>
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AnAoxue Huang\* Vifeng Xiong\*<br>
1353227546@qq.com 327988214@qq.com<br>
Xiangshui Miao\* Xingsheng Wang\*†<br>
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Yifeng Xiong\*<br>
327988214@qq.com<br>
Xingsheng Wang\*<sup>†</sup><br>
xswang@hust.edu.cn<br>
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1575803685@qq.com

2741105136@qq.com

1353227546@qq.com

miaoxs@hust.edu.cn

327988214@qq.com

xswang@hust.edu.cn

**Multi-order Differential Neural Network for TCAD Simulation of**<br>
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Zifei Cai<sup>\*</sup> AnAoxue Huang<sup>\*</sup> Yifeng Xiong\*<br>
1575803685@qq.com<br>
Dejiang Mu<sup>\*</sup> Xiangshui Miao<sup>4</sup> 27998214@qq.com<br>
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15758036858@qq.com<br>
Dejiang Mu<sup>\*</sup> Xingshui Miao<sup>\*</sup> Xingsheng Wang<sup>\*†</sup><br>
27411 **Multi-order Differential Neural Network for TCAD Simulation of**<br> **the Semiconductor Devices**<br>
Zifei Cai\* AnAoxue Huang<sup>\*</sup> Yifeng Xiong<sup>\*</sup><br>
1575803685@qq.com<br>
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Dejiang Mu\* Xiangshui Miao\* Xingsheng Wang\*1<br>
2778803685@gap.com<br>
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2727988214@<sub>99</sub>q.com<br>
2727988214@<sub>99</sub>q.com<br>
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**ABSTRACT** These studies specifically include the use of trained Multilayer<br>Perceptron (MLP) models to predict device current-voltage (I<sub>D</sub>-V<sub>G</sub>) Technology Computer Aided Design (TCAD) is a crucial step in **Multi-order Differential Neural Network for TCAD Simulation of**<br>  $\text{the Semiconductor}$  Devices<br>  $\text{Zifici Cai*}$ <br>  $\text{1575803685@eqq.com}$ <br>  $\text{Dejiang Mat*}$ <br>  $\text{1575803685@eqq.com}$ <br>  $\text{Dejiang Mat*}$ <br>  $\text{2741105136@qq.com}$ <br>  $\text{Dejiang Mat*}$ <br>  $\text{2741105136@qq.com$ **Multi-order Differential Neural Network for TCAD Simulation of**<br> **the Semiconductor Devices**<br>
Zitei Cai\* And oxus Huamg\* Yifeng Xiong\*<br>
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1575803685@qq.com<br>
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Zifei Cai\* AnAoxue Huang\* Yifeng Xiong\*<br>
1575803685@qq.com<br>
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Ultang\* Yifeng Xiong\*<br>
27988214@qq.com<br>
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Miao\* Xingsheng Wang\*<br>  $^{*}$ <br>  $^{*}$ <br>  $^{*}$ <br>  $^{*}$ <br>  $^{*}$ <br>  $^{*}$ <br>  $^{*}$ **Example 1.2**<br> **Example 1. Example 18 The Spatial Markon Constant of the spatial distribution of physical quantities with the spatial d Example 18 Simulation of**<br> **Summary**<br> **Such as devices**<br> **Sugarcom**<br> **Sugarcom**<br> **Sugarcom**<br> **Summary**<br> **Summary**<br> **Summary**<br> **Summary**<br> **Summary**<br> **Summary**<br> **Summary**<br> **Summary**<br> **Summary**<br> **Perceptron (MLP) models to Example 18 The Simulation of**<br> **Conceptions**<br> **Conception**<br> **Conce Example 18 The realist School Simulation of the realistic state of the realist state of the realist**  $\frac{27}{988214\omega qq, \text{com}}$  **Miao\* Singsheng Wang\*\***  $\alpha$ **.edu.cn and the section of the section of the section of the state o** simulation results of traditional TCAD tools, such as finite **Example 18 CONSTRON Simulation of COVICES**<br>
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Miao \* Xingsheng Wang \* 1<br>
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neutral of the burnter solutions and finite dentation states and the spin of concludes the paper and provides an entired of PINN is a burnd new mumeral solution paradigm [6.7]. The basis for the MDN is a burndom paper and compared to the initire via the method and time electric problem in Machine Learning-TCAD.<br>
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condition In this paper, we introduce a Multi-order Differential Neuval<br>Network (MDNN) model and associated simulation and<br>optimization algorithms for the self-consistent solution of<br>Poisson's equation and drift-diffusion equations optimization algorithms for the self-consistent solution of the self-consistent solution<br>Poisson's equation and drift-diffusion equations under steady-state<br>conditions. By replacing the deep fully connected neural network<br> (DNN) used in traditional PINN methods with a composite MDNN model, we obtain a novel machine learning approach for solving coupled Poisson's equation and carrier transport equations.<br>The structure of this paper is as foll MDNN model, we obtain a novel machine learning approach for solving coupled Poisson's equation and carrier transport covaring coupled Poisson's equation and carrier transport covaring coupled Poisson's equation and carrier Solving coupled Poisson's equation and carrier transport<br>
Solving coupled Poisson's equation and carrier transport<br>
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a detailed description of the mathema structure of this paper is as follows: In Section 2, we provide<br>equations.<br>The structure of this paper is as follows: In Section 2, we provide<br>a detailed description of the mathematical formulation of MDNN,<br>diodes using MD The structure of this paper is as follows: In Section 2, we provide<br>a detailed description of the mathematical formulation of MDNN,<br>the process of performing numerical simulations of PN junction<br>diodes using MDNN, and the in plotes or penoming inimetrical simulations or 11y junction<br>diodes using MDNN, and the accuracy improvement algorithm<br>based on the Residual Neural Network (Res-Net) concept. In<br>Section 3, we present numerical simulation the most stars of the actuate of the control of the control and soles of the Residual Neural Network (Res-Net) concept. In<br>Section 3, we present numerical simulation results of PN junction<br>diodes under various conditions, asset on the cessual "stewath" chearter concept. The conception and a becoming Section 3, we present numerical simulation results of PN junction diodes under various conditions, the gradient descent process of diodes under

## **PROCESS**

# Model

becomin , we pressed matrixed simulation resumes or 1 x planeting<br>diodes under various conditions, the gradient descent process of<br>the loss function, and compare the carrier and the potential<br>distributions obtained throug fluores inducts vanions, the gradient execution (we shall distributions obtained through MD-PINN simulation with the corresponding simulation results from Sentauraus TCAD. The creatist demonstrate that the improved RBFNN the cost interior and complete the carrier dare to the potential<br>distributions obtained through MD-PINN simulation with the<br>corresponding simulation results from Sentaurus TCAD. The<br>results demonstrate that the improved R usholutions concared uniongly *with*- interaction corresponding simulation results from Schatzants TCAD. The results demonstrate that the improved RBFNN model has the creation 4 concludes the paper and provides an outlook concessorially dimagramianta increases from Scalars is created the improved RBFNN model has the capability to accurately simulate semiconductor devices. Finally, Section 4 concludes the paper and provides an outlook on fu considerable that we may be explored to the model and the respect to the model and capability to accurately simulate semiconductor devices. Finally, Section 4 concludes the paper and provides an outlook on future research nconductor devices. Finally,<br>
sovides an outlook on future<br> **ND SIMULATION**<br>
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mensional case,<br>
sit of five output terms: u.  $u^{(1)}$ ,  $u^{(2)}$ ,  $u^{(3)}$ ,  $u^{(4)}$ . Among them  $u^{(1)}$ ,  $u^{(2)}$ ,  $u^{(3)}$ ,  $u^{(4)}$  are the first to fourth-order partial Machine Learning-TCAD.<br> **RAL NETWORK AND SIMULATION**<br>
Machine Learning-TCAD.<br> **RAL NETWORK AND SIMULATION**<br> **CESS**<br>
com, we will provide a detailed description of the Multi-order Differential Neural Network Model<br>
and the **L. NETWORK AND SIMULATION**<br> **L. NETWORK AND SIMULATION**<br>
S. we will provide a detailed description of the<br>
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the specific process of utilizing MDNN for the<br>
miconductor devices.<br> Learning-TCAD.<br> **ETWORK AND SIMULATION**<br>
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or devices.<br> **fferential Neural Networ** research in Machine Learning-TCAD.<br> **2 NEURAL NETWORK AND SIMULATION**<br> **PROCESS**<br>
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In this section, we will provide a detailed description of the<br>
proposed Multi-order Differential Neural Network Model<br>
(MDNN) and the specific process of utilizing MDNN for t **PROCESS**<br>In this section, we will provide a detailed description of the<br>proposed Multi-order Differential Neural Network Model<br>(MDNN) and the specific process of utilizing MDNN for the<br>simulation of semiconductor devices **FROCESS**<br>In this section, we will provide a detailed description of the<br>proposed Multi-order Differential Neural Network Model<br>(MDNN) and the specific process of utilizing MDNN for the<br>simulation of semiconductor devices In this section, we will provide a detailed description of the<br>proposed Multi-order Differential Neural Network Model<br>(MDNN) and the specific process of utilizing MDNN for the<br>simulation of semiconductor devices.<br>2.1 **Mul** proposed Multi-order Differential Neural Network Model<br>(MDNN) and the specific process of utilizing MDNN for the<br>simulation of semiconductor devices.<br> **2.1 Multi-order Differential Neural Network Model**<br>
The Multi-order D

Multi-order Differential Neural Network for TCAD Simulation of the Semiconductor Devices<br>
bandwidth parameters w and kernel function centers b. For the<br>
bandwidth parameters w and kernel function centers b. For the<br>
measu their own distinct adaptive kernel functions:  $f_1(t)$ ,  $f_2(t)$ ,  $f_3(t)$ , functions to approximate the numerical solution of carrier  $f_4(t)$ ,  $f_5(t)$ . In order to make the five output terms of the MDNN model satisfy the required mathematical relationships, we Forder Differential Neural Network for TCAD Simulation of the Semiconductor Devices<br>
Under Differential Neural Network for TCAD Simulation of the Semiconductor Devices<br>
Unter apply the property of neurons in the hidden la

$$
f_1(t) = \frac{\sqrt{\pi} \, \text{terf}(t) + e^{-t^2}}{2w^2} \tag{1}
$$

$$
f_2(t) = \frac{\sqrt{\pi} \, erf(t)}{2w} \tag{2} \quad \text{order.}
$$

$$
f_3(t) = e^{-t^2} \tag{3}
$$

$$
f_4(t) = -2wte^{-t^2} \tag{4}
$$

$$
f_5(t) = 2w^2(2t^2 - 1)e^{-t^2}
$$
 (5)

 $f_1(t) = \frac{\sqrt{\pi} \tan t/(1) + e^{-t^2}}{2\pi^2}$  (1) that numerical directions computation computation computations  $f_2(t) = \frac{\sqrt{\pi} \tan t/(1)}{2\pi}$  (1) this worth noting that the five output quantities  $f_3(t) = -2Wte^{-t^2}$  (3) the sole of pro  $f_2(t) = \frac{\sqrt{\pi} e f(t)}{2w}$  (2) one the physical quantities is the second in the second of the section of the second in the second in the section of the second transmission in the section of the control of  $f_3(t) = 2w^2(2t^2 -$  $J_3(1) = e^{i\theta}$  (3)  $\ln \left( \frac{1}{2} \right)$  and the two coupled that the constructed the external in the subsequent device similar the subsequent of  $f_3(t) = 2w^2(2t^2 - 1)e^{-t^2}$  (4) meass. Due to the mathematical relationships progresses. Here,  $t$  ( $t = w(x - b)$ ) represents the input to the divergence of charge density. The distributed moreoton in the hidden layer neurons,<br>
simulations.<br>
And erf (f) denotes the Graussian error function.<br>
And erf ( kernel function function) in the bidden layer namos,<br>
simulations. For possing the relation function and are proper of the same type of desi and  $\sigma r f(t)$  denotes the Gaussian error function.<br>
Addibitionally, the hidden layer on the MDNN  $\Delta t$  and the output layer on the MDNN  $\Delta t$  and  $\sigma t$  can be considered and to every the simulation of the section model are Additionally, the hidden layer and the output layer of the MDNN<br>
Additionally, the hidden layer (i.e., having the same type of dealative kernel<br>
michalden are fit (a) connected all neurons of the same type in the entire h model are not fully connected. All neurons of the same type in the sum is to constrain to be about in TCAD for samiconductor device<br>
dined in every  $\left(\frac{1}{16}\right)$ , having the same type of adaptive kemel<br>
dined in the comp

$$
u = \sum_{i=1}^{n} A_i \left( \frac{\sqrt{\pi} w_i (x - b_i) erf(w_i (x - b_i)) + e^{-w_i^2 (x - b_i)^2}}{2w_i^2} \right)
$$
(6) 
$$
\epsilon \frac{d^2 \psi}{dx^2} = -\frac{\epsilon^2 \psi}{w_i^2}
$$

$$
u^{(1)} = \sum_{i=1}^{n} A_i \left( \frac{\sqrt{\pi} \operatorname{erf}(w_i(x - b_i))}{2w_i} \right) \tag{7}
$$

$$
u^{(2)} = \sum_{i=1}^{n} A_i \left( e^{-w_i^2 (x - b_i)^2} \right)
$$
\n(8)\n
$$
u^{(3)} = \sum_{i=1}^{n} A_i \left( -2w_i^2 (x - b_i) e^{-w_i^2 (x - b_i)^2} \right)
$$
\n(9)\nIn the equations,  $\psi, n$ ,

$$
u^{(3)} = \sum_{i=1}^{n} A_i \left( -2w_i^2 (x - b_i) e^{-w_i^2 (x - b_i)^2} \right)
$$
 (9)

$$
u^{(4)} = \sum_{i=1}^{n} A_i \left( 2w_i^2 \left( 2w_i^2 (x - b_i)^2 1 \right) e^{-w_i^2 (x - b_i)^2} \right)
$$
 (10) charge density. c is  
impurities in the devic

Multi-order Differential Neural Network for TCAD Simulation of the Semiconductor Devices **DAC'24**, June 23–27, 2024, San Francisco, CA, USA<br>
bandwidth parameters w and kernel function centers b. For the results with fewer Multi-order Differential Neural Network for TCAD Simulation of the Semiconductor Devices<br>
bandwidth parameters w and kernel function centers *b*. For the results with fewer training iterations. Secondly, single-layer<br>
out Multi-order Differential Neural Network for TCAD Simulation of the Semiconductor Devices<br>
DAC<sup>22</sup>4, June 23–27, 2024, San Francisco, CA, USA<br>
bandwidth parameters w and kernel function centers b. For the<br>
output layer als Multi-order Differential Neural Nework for TCAD Simulation of the Semiconductor Devices<br>
bandwidth parameters w and kernel function centers b. For the results with fewer training iterations. Secondly, single-layer<br>
output Multi-order Differential Neurol Nework for TCAD Simulation of the Semicondator Devices DAC<sup>-24</sup>, June 23-27, 2024, San Francisco, CA, USA<br>bandwidth parameters w and kernel function centers *b*. For the results with fewer Multi-ordsr Differential Network for TCAD Simulation of the Semiconductor Devices<br>
bandwidth parameters w and kernel function centers *b*. For the<br>
benduction similar to the same group of neurons in the hidden layer also s of the Semiconductor Devices<br>
DAC'24, June 23-27, 2024, San Francisco, CA, USA<br>
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algoer also shares neural networks have stronger interpret miconductor Devices<br>
DAC'24, June 23-27, 2024, San Francisco, CA, USA<br>
5. For the results with fewer training iterations. Secondly, single-layer<br>
Ilso shares neural networks have stronger interpretability, lower training<br> differential Network for TCAD Simulation of the Semicondator Devices<br>
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parameters w and kernel function centers *b*. For the<br>
r, each group of neutrons in the hidden layer a Mali-order Differential Nearly Newsthet TCAD Simulation of the Scatisson<br>devote by DAC24, June 23-27, 2024, Sun Function, CA, USA<br>bandwidth parameters w and kernel function centers b. For the results with fewer training i Matis ender Differential Nearal Network for TCAD Simulation of the Simison<br>dates the mathematical Forms in the hidden hayer also shares and the mathematical forms of the mathematical forms of the mathematical forms of the Multi-sender Differential Neratal Neratal Simulation of the Semiconductor Devices<br>
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bandwidth parameters w and kernel function centers b. For the<br>
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of neurons in the hidden layer also shares neural networks have stronger i (2) order. ial Neuvolt for TCAD Simulation of the Semiconductor Devices<br>
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meters w and kernel function centers b. For the results with fewer training iterations,<br>
the progress of the coupled analytic and so shares<br>
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22 + 10  $\approx$  22, 2024, Sam Francis<br>
22 + 10  $\approx$  22, 2024, Sam Francis<br>
23 of the curbut layer ates shares neural networks have Motive or Differential Nearl Stewet for TCAD Samulation of the Samiconbaton Devices<br>
bandwidth parameters w and kernel function centers *b*. For the<br>
coupler layer training iterations. Secondly, single-layer<br>
backnot band Muti ceder Differential Smull Memoir for TCAD Simulation of the stension<br>baraboidh parameters w and kennel function earters  $h$ . For the results with frever training iterations, Secondly, single-layer<br>output layer, each g Multi coder Differestial Neural bandwidth parameters w and kennel function centers  $h$ . For the results with fever training iterations. Secondly, single-layer<br>outer layer, each agree of reconversion the hidden hyer is the interaction and a stronger inte handwidth parameters w and kernel function centers b. For the results with fever training iterations. Secondly, single-layer the same vection of the finden layer is the distribution for the same of the same of the same of and the particle is the same of the control in the hidden have the bothes from the same of control in the same of Are Amovwhile, the hidese To required in the hidden layer and required in the output layer and the output layer and the single in the single controllation of the output layer and the output in the single controllation of all set to zero. The only difference among these free neurons, in datine, we hope to use advantage of the same prop in the hidden layer is that they exch have connected are interestingential set of causas in the same prop with the same eyenp in the bidden layer is that they each bave excellent smoothness and fitting expactificant<br>between layer in the same type of having expective materials of Caretist<br>A(1, f<sub>2</sub>(t), f<sub>2</sub>(t), f<sub>2</sub>(t), f<sub>2</sub>(t DAC'24, June 23–27, 2024, San Francisco, CA, USA<br>results with fewer training iterations. Secondly, single-layer<br>neural networks have stronger interpretability, lower training<br>computational costs, and require fewer overall DAC'24, June 23-27, 2024, San Francisco, CA, USA<br>results with fewer training iterations. Secondly, single-layer<br>neural networks have stronger interpretability, lower training<br>computational costs, and require fewer overall DAC'24, June 23-27, 2024, San Francisco, CA, USA<br>results with fewer training iterations. Secondly, single-layer<br>neural networks have stronger interpretability, lower training<br>computational costs, and require fewer overall DAC'24, June 23-27, 2024, San Francisco, CA, USA<br>results with fewer training iterations. Secondly, single-layer<br>neural networks have stronger interpretability, lower training<br>computational costs, and require fewer overall DAC'24, June 23-27, 2024, San Francisco, CA, USA<br>results with fewer training iterations. Secondly, single-layer<br>neural networks have stronger interpretability, lower training<br>computational costs, and require fewer overall DAC'24, June 23-27, 2024, San Francisco, CA, USA<br>results with fewer training iterations. Secondly, single-layer<br>neural networks have stronger interpretability, lower training<br>computational costs, and require fewer overall DAC'24, June 23-27, 2024, San Francisco, CA, USA<br>results with fewer training iterations. Secondly, single-layer<br>neural networks have stronger interpretability, lower training<br>computational costs, and require fewer overall DAC'24, June 23-27, 2024, San Francisco, CA, USA<br>results with fewer training iterations. Secondly, single-layer<br>neural networks have stronger interpretability, lower training<br>computational costs, and require fewer overall DAC24, June 23-27, 2024, San Francisco, CA, USA<br>results with fewer training iterations. Secondly, single-layer<br>neural networks have stronger interpretability, lower training<br>computational costs, and require fewer overall n DAC<sup>24</sup>, June 23-27, 2024, San Francisco, CA, USA<br>results with fewer training iterations. 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Secondly, single-layer<br>neural networks have stronger interpretability, lower training<br>computational costs, and require fewer overall DAC<sup>24</sup>, June 23-27, 2024, San Francisco, CA, USA<br>results with fewer training iterations. Secondly, single-layer<br>neural networks have stronger interpretability, lower training<br>computational costs, and require fewer overall DAC'24, June 23-27, 2024, San Francisco, CA, USA<br>results with fewer training iterations. Secondly, single-layer<br>neural networks have stronger interpretability, lower training<br>computational costs, and require fewer overall DAC'24, June 23-27, 2024, San Francisco, CA, USA<br>results with fewer training iterations. Secondly, single-layer<br>neural networks have stronger interpretability, lower training<br>computational costs, and require fewer overall DAC'24, June 23-27, 2024, San Francisco, CA, USA<br>results with fewer training iterations. Secondly, single-layer<br>neural networks have stronger interpretability, lower training<br>computational costs, and require fewer overall DAC'24, June 23-27, 2024, San Francisco, CA, USA<br>results with fewer training iterations. Secondly, single-layer<br>neural networks have stronger interpretability, lower training<br>computational costs, and require fewer overall DAC'24, June 23-27, 2024, San Francisco, CA, USA<br>results with fewer training iterations. Secondly, single-layer<br>neural networks have stronger interpretability, lower training<br>computational costs, and require fewer overall results with fewer training iterations. Secondly, single-layer<br>results with fewer training iterations. Secondly, single-layer<br>results have stronger interpretability, lower training<br>computational costs, and require fewer o results with fewer training iterations. Secondly, single-layer neural networks have stronger interpretability, lower training computational costs, and require fewer overall network parameters. In addition, we hope to take computational costs, and require lever or overall network<br>parameters. In addition, we hope to take advantage of the<br>excellent smoothness and fitting capabilities of Gaussian basis<br>functions to approximate the unmerical sol Excellent smoothness and fitting capabilities of Gaussian basis<br>excellent smoothmess to approximate the numerical solution of carrier<br>concentration distribution with steep gradients in space [15].<br>Finally, our design ensu

It is worth noting that the five output quantities of the neural network model proposed in this paper have realistic physical their connection of the interest of the functions  $f_1(t) = \frac{\sqrt{\pi}t}{2}$  (b),  $f_2(t)$ ,  $f_3(t)$ , the order to make the free output terms of the connected only the reality there is a specific output term in the connected only  $f_2(t) = \frac{\sqrt{\pi} \, e(t)}{2}$ . In order to make the five output term soft the mate of the neural that the properties are and  $\pi$  output term of the neural term of the neural term of the neural term of the neural term of the ne MDNN model satisfy the required manthematical region contribute in the case of the area in the same of the sum of the outp choos the multimorial forms of these adjoints in the same the same interded in the same is to be a single text of its computation of its computation of the same single  $f_1(t) = \frac{\sqrt{\pi} \exp(t) + e^{-t^2}}{2\pi}$  (1) that numerical di to be as follows after extensive numerical experiments:<br>
amount of numerical differentiation computation has the searches<br>  $f_1(t) = \frac{\sqrt{\pi} \exp(e^{t})e^{-t}}{2\pi t}$  (1) that numerical errors generated during the computation by the <sup>4*e*-r<sup>2</sup> (1) that numerical errors generated during the computa<br>
are not progressively amplified with the increase i<br>
22 order.<br>
(3) It is worth noting that the five output quantities o<br>
(4) meanings in the subsequent d</sup> 1.<br>
(1) that numerical errors generated during the computation<br>
are not progressively amplified with the increase in de<br>
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nextwork model proposed i (1) that numerical errors generated during the computation proces<br>
(2) order.<br>
(2) order.<br>
(3) this worth noting that the five output quantities of the neu<br>
(4) meanings in the subsequent device simulation and solution<br>
( simulations. functions to approximate the numerical solution of carrier concentration distribution with steep gradients in space [15].<br>Finally, our design ensures the analyzability of the MDNN, allowing for efficient and accurate calc concentration distribution with steep gradients in space [15].<br>Finally, our design ensures the analyzability of the MDNN,<br>allowing for efficient and accurate calculation of its output results<br>various orders of partial der Finally, our design ensures the analyzability of the MDNN,<br>Ellowing for efficient and accurate calculation of its output results<br>allowing for efficient and accurate calculation of its output results<br>various orders of part showing for efficient and accurate calculation of its output results<br>allowing for efficient and accurate calculation of its output results<br>various orders of partial dierivatives. This not only avoids a large<br>anount of num where the word that we wall derivative strates the condition of the sequence of partial derivatives. This not only avoids a large amount of numerical differentiation computation but also ensures that numerical errors gene simulation is how the specific material differentiation computation but also ensures<br>that numerical differentiation computation but also ensures<br>that numerical errors generated during the computation process<br>order.<br>It is and the multimoreal energy and the method of the method in the method of the method that numerical errors generated during the computation process<br>are not progressively amplified with the increase in derivative<br>order.<br>It oting that the five output quantities of the neural<br>
lel proposed in this paper have realistic physical<br>
the subsequent device simulation and solution<br>
to the mathematical relationships between these five<br>
only need to mu el proposed in this paper have realistic physical<br>the subsequent device simulation and solution<br>the mathematical relationships between these five<br>only meed to multiply them by specific constants to<br>five physical quantitie 1 this paper have realistic physical<br>th device simulation and solution<br>tical relationships between these five<br>ultiply them by specific constants to<br>ultiply them by specific constants to<br>ty, gradient of charge density, and extra fraction and solution<br>simulation and solution<br>ships between these five<br>m by specific constants to<br>1 space: potential, electric<br>t of charge density, and<br>istribution of these five<br>sult of interest in TCAD<br>**S**<br>**S**<br>**S**<br>

the mathematical relationships between these five<br>the mathematical relationships between these five<br>inpixed quantities in space: potential, electric<br>charge density, gradient of charge density, and<br>charge density. The di ical relationships between these five<br>cical relationships between these five<br>ultiply them by specific constants to<br>untities in space: potential, electric<br>y, gradient of charge density, and<br>y. The distribution of these fiv busing the vector these five<br>ships between these five<br>n by specific constants to<br>space: potential, electric<br>of charge density, and<br>stribution of these five<br>ult of interest in TCAD<br>for semiconductor device<br>sistent solution process. Due to the mathematical relationships between these five<br>
equantities, we only need to multiply them by specific constants to<br>
represent the five physical quantities in space: potential, electric<br>
divergence of c quantities, we only readed to multiply them by specific constants to<br>represent the five physical quantities in space: potential, electric<br>field strength, charge density, gradient of charge density, and<br>divergence of charg

$$
\varepsilon \frac{d^2 \psi}{dx^2} = -\rho = q(n-p-c) \tag{11}
$$

$$
D_p \frac{d^2 p}{dx^2} + \mu_p \frac{dp}{dx} \cdot \frac{d\psi}{dx} + \mu_p p \frac{d^2 \psi}{dx^2} = 0
$$
 (12)

$$
D_n \frac{d^2 n}{dx^2} - \mu_n \frac{dn}{dx} \cdot \frac{d\psi}{dx} - \mu_n n \frac{d^2 \psi}{dx^2} = 0
$$
 (13)

(i)-(i), we represent the method quantities in space. The distribution is the method of the method and interest in the distribution is pace. Political state here are the five physical quantities in space. Political stat In the equations,  $\psi$ , *n*, *p* represent the three variables to be solved: potential, electron concentration, and hole concentration.  $\rho$  is the neural network training process<br>
b) in presents the input of the divergence of charge density, The distribution of the<br>
hol) in the hidden layer neurons,<br>
b) in the hidden layer neurons,<br>
and the output layer of the MDN ) epresents the input in the divergence of charge density. The distribution of these five<br>or function.<br>
Simulations are the MDNN of the stellar distribution of these five<br>or function.<br>
the output layer of the MDNNN one th hidden layer (i.e., having the same type of datapitive kurell the core probable to severe in the content of the content of the energy of a datable are as follows: Firstly, through the two sets in the content are as for th function) ine connected only to a pecific ouprigrom in the simulation is bow to anisotropic multiple numerical experiments, we have the simulation of the simulation of the experiments of the found that compared that compa output layer. In other words, each output is more in the area in comparison that is a monotonic layer and the single-layer of the position of the position of the properties in the single-layer. As a result, we choose to u network inspirse the linear vecipates in the output results of [10]. Here, we choose to use the Change of trap contents the computer of the contents of the contents of the same type in the hidden hyer. As a result, we spe all normals of the same type in the bidden layer. As a result, we converging the model intermediate and entropies of the same the model of the converging to the SMN reduced MDNNtu,  $u^{(1)} = \sum_{i=1}^{n} A_i \left( \frac{\sqrt{\pi} e(r - b_i) \pi^2 ($ represent the twe physical quantitus in space: potential, electric steps<br>the distringth, charge density, gradient of charge density, and<br>divergence of charge density. The distribution of these five<br>physical quantities is held strength, charge density, gradient of charge density, and divergence of charge density. The distribution of these five<br>by physical quantities is precisely the result of interest in TCAD<br>simulations.<br>2.2 Device Simula divergence of charge density. The distribution of these tive<br>ghysical quantities is precisely the result of interest in TCAD<br>simulations.<br>2.2 Device Simulation Process<br>The core problem to be solved in TCAD for semiconduct physical quantities is precisely the result of interest in ICAD<br>
simulations.<br> **2.2 Device Simulation Process**<br>
The core problem to be solved in TCAD for semiconductor device<br>
simulation is how to achieve self-consistent simulations.<br>
2.2 Device Simulation Process<br>
The core problem to be solved in TCAD for semiconductor device<br>
simulation is how to achieve self-consistent solutions for the<br>
coupled electric field equations and carrier tra **2.2 Device Simulation Process**<br>The core problem to be solved in TCAD for semiconductor device<br>simulation is how to achieve self-consistent solutions for the<br>coupled electric field equations and carrier transport equation The core problem to be solved in TCAD for semiconductor device<br>simulation is how to achieve self-consistent solutions for the<br>coupled electric field equations and carrier transport equations<br>[16]. Here, we choose to use t simulation is how to achieve self-consistent solutions for the coupled electric field equations and carrier transport equations (16). Here, we choose to use the Poisson equation to describe the spatial distribution of the coupled electric field equations and carrier transport equations<br>
[16]. Here, we choose to use the Poisson equation to describe the<br>
spailal distribution of the potential and the derift-diffusion equation<br>
under steady-st [16]. Here, we choose to use the Poisson equation to describe the papal alistbution of the potential and the drift-diffusion equation<br>spaid alistbution of the potential and the drift-diffusion equation<br>much estedy-state c example state conditions as the carrier transport equation<br>spatial distribution of the potential and the drift-diffusion equation. The<br>specific mathematical forms of these two types of equations in<br>one-dimensional cases a under steady-state conditions as the carrier transport equation. The<br>specific mathematical forms of these two types of equations in<br>one-dimensional cases are described as follows:<br> $\epsilon \frac{d^2 \psi}{dx^2} = -\rho = q(n - p - c)$  (11)<br> $D_p \frac{$ 



The left diagram (3.a) illustrates the schematic of the combined MDNN model used for<br>equations, while the right diagram (3.b) represents the specific process of training the co<br>equations, while the right diagram (3.b) rep

follows:

$$
\psi = q (u_n - u_p - u_c) / \varepsilon + Ax + B \tag{14}
$$

$$
\mathcal{E} = -\frac{d\psi}{dx} = -q\left(u_n^{(1)} - u_p^{(1)} - u_c^{(1)}\right)/\varepsilon + A
$$
 (15) local optimum. The v  
quickly decrease to a

$$
n = u_n^{(2)} \quad p = u_p^{(2)} \quad c = u_c^{(2)} \tag{16}
$$

$$
\frac{dn}{dx} = u_n^{(3)} \qquad \frac{dp}{dx} = u_p^{(3)}
$$
 (17) choose to train Model?

and the dimension of the deteric field is always stirtly and the basic of a such as determined by the output terms of the three MDNN models is mathed, originating from the basic ideal of the such as dependent, and carrier

**Example 18**<br> **Example 18)**<br> **Example 18) Model Properties the schematic of the combined MDNN model used for self-consister<br>
agram (3.b) represents the specific process of training the combined MD<br>
while the right diagram (3.b) represents the specific process of Example 1997**<br> **Example 1997**<br> **Example 1997**<br> **Example 11)**<br> **Example 11)**<br> **Example 11)**<br> **Example 11)**<br> **Example 11)**<br> **Example 11)**<br> **Example 12)**<br> **Example 12)**<br> **Example 12)**<br> **Example 12)**<br> **Example 12)**<br> **Example** Figure 3: The left diagram (3.4) illustrates the schematic of the combined MDNN model used for self-consistent solution of coupled<br>by shock equations, while the right diagram (3.6) represents the specific process of train Gradient Content of the basic in the basic in the discussion of the discussion of the basic in the content of the property of the contentration, and hole conc (Physical MDNN model used for self-consistent solution of coupled<br>
Mines Internal Network)<br>
The Consumer Strain of Coupled<br>
The process of training the combined MDNN model according<br>
esimulation.<br>
number of physical quanti **Example 12**<br>
For the Games of training the conbined MDNN model according<br>
Find process of training the combined MDNN model according<br>
simulation.<br>
Experimentation properties for the experimental in the TCAD<br>
simulation p Simultaneously in parallel, the model of the model interferometrian process of training the combined MDNN model according esimulation.<br>
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simulation rocess from three (electric potential, electron<br>
concentration **Example 10:30**<br>
The **Consulation**<br>
Index **MDNN** model used for self-consistent solution of coupled<br>
iffic process of training the combined MDNN model according<br>
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number of physical quantities to be determined The process of training the complete of the complete training process of training the combined MDNN model according and multion process of training the combined MDNN model according number of physical quantities to be dete The **Conser Consert Consert Consert Consert Solution** of coupled<br>
iffic process of training the combined MDNN model according<br>
e simulation.<br>
number of physical quantities to be determined in the TCAD<br>
simulation process **Course**<br> **C** ined MDNN model used for self-consistent solution of coupled<br>tific process of training the combined MDNN model according<br>e simulation.<br>number of physical quantities to be determined in the TCAD<br>simulation process from thr ined MDNN model used for self-consistent solution of coupled<br>effic process of training the combined MDNN model according<br>e simulation.<br>number of physical quantities to be determined in the TCAD<br>simulation process from thre

Therefore, we draw inspiration from the Gummel method and Figure 3: The left diagram at Ga) illustrates the securities of the combined MDNN model are of diagram (3.b) perpeneuts the specific process of praining the combined MDNN model according<br>to the optimization algorithm prop by sying tequations, while the regard the present in performance consistents the present of the electric present of the perform proposed in this paper device in mather of physical quantities to be determined in the TCAD a to the optimuzation algorithm proposed in this paper to achieve device simulation.<br>
approximate the distributions of net impuriby concertation, doncer mainly concertation, and acceptor impurily concertation, and the solvi approximate the distributions of net impurity concentration, donor<br>nimather of physical quantities to be determined in the TCAD<br>physical distribution and acceptor impurity concentration in the simulation potents from thre approximate the distributions of net intervention (11) with the control of the equation of the control equation (11) the control equation (11) with the simulation (11) with the control of the control of the control of the mpairies concentration, and secretor mappied vectors have a summation in the summation concentration in the section potential, election and have a summit and the internal parameters respectively.<br>
The notation and paramet device as initial twist best we first between the content of the specific controlled here. The specific value incrementation and here coefficients are the specific values of the specific values of the specific values of t that is increased by the system transmission costant throughout the computer system contrast in a metally and Model P. as electron and hole concentration and hole concentration. The metallic is the unit task is to hole an subsequent processes. We then utilized the coupling terms of Model N and Model P and Model P and Model P and Consequently, physical quantities such as electric potential, (19del N and V and Nord P and Consequently, physic Consequently, physical quantities and he activite potential of statisty the control equation (12) and determined the propriet of the statisty control equation scentiling propriet to perform a control of the statistic perf electric field intensity, contration concentration, concentration, concentration, concentration, the energy as in a such as the respective by utilizing the gradient-descent<br>represented by the output terms of the three MDN ific process of training the combined MDNN model according<br>
esimulation.<br>
number of physical quantities to be determined in the TCAD<br>
simulation process from three (electric potential, electron<br>
concentration, and hole con **e simulation.**<br> **Examplementation** process from three (electric potential, electron<br>
simulation process from three (electric potential), as required by the<br>
currently used Newton-Raphson and Gummel methods, to two<br>
celect number of physical quantities to be determined in the TCAD simulation process from three (electric potential, electron concentration, and hole concentration), as required by the currently used Newton-Raphson and Gumentl me number of physical quantities to be determined in the TCAD<br>simulation process from three (electric potential, electron<br>concentration, and hole concentration), as required by the<br>currently used Newton-Raphson and Gummel met simulation process from three (electric potential, electron<br>concentration, and hole concentration), as required by the<br>currently used Newton-Raphson and Gummel methods, to two<br>cleetron concentration and hole concentration) concentration, and hole concentration), as required by the currently used Newton-Raphson and Gumenle methods, to two cleletron concentration and hole concentration).<br>The next task is to make the output distribution of Mode currently used Newton-Raphson and Gummel methods, to two<br>
(electron concentration and hole concentration).<br>
The next task is to make the output distribution of Model P and<br>
Model N satisfy the control equation (12) and con The next task is to make the output distribution of Model P and<br>Model N satisfy the control equation (12) and control equation<br>(13), as well as their respective boundary conditions. Overall, we<br>aim to achieve this objecti Free most unas the winner to expect the excessive product of model. N satisfy the control equation (12) and control equation (13), as well as their respective boundary conditions. Overall, we (13), as well as their respec Model N anatsly the control equation (12) and control equation (12) and control equations. Overall, we aim to achieve this objective boundary orditions. Overall, we aim to achieve this objective by utilizing the gradient-(13), as well as their respective boundary conditions. Overall, we are<br>nit to achieve this objective by utilizing the gradient-descent emethod, originating from the basic idea of the PINN<br>(Physics-Informed Neural Network)





Figure 4: Schematic diagram of the insparing of stribution in Figure 6: Schematic diagram of the simulation results of<br>  $\frac{1}{2}$ <br>  $\$ Figure 4: Schematic diagram of the impurity distribution in Figure 6: Schematic diagram of the simulation results of<br>  $\frac{1}{1}$ <br>  $\frac{$ smaller the PN junction diode to be simulated.<br>
<br>
Figure 5. Schematic discussions of the MDNN composite model during the<br>
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Figure 5. Schematic discussions of the MDNN composite model during the<br>
Figure 5. Schematic discus **Example model N, model P) to obve the residual content model distribution of the Simulation of the Nighter set is found to the Nighter of the** value of the loss function remains unchange in the loss function remains of the loss function remains uncertainty and the loss function remains uncertainty and  $\frac{1}{2}$  and  $\frac{1}{2}$  and  $\frac{1}{2}$  and  $\frac{1}{2}$  and  $\frac{1$ Figure 5: Schematic diagram and number of descents in the base of gradient state of the simulation of the FN junction diagram of the simulation of the NS incomes and the MS incomes and the MS incomes and  $\frac{1}{2}$  and  $\frac$ Figure 5. Schematic dispared and the changes in the base of the respectively, and the residual of the residual of the fixed simulation of the simulation residual of the Figure 3. Schematic dispared in the changes in the c Figure 5: Schematic diagram and the changes in the loss Figure 7: Schematic diagram of the simulation results of Figure 7: Schematic diagram of the simulation results of Figure 7: Schematic diagram of the simulation resul **Example 1.1**<br> **Example 1.** Figure 5: Schematic diagram of the changes in the base<br>
Figure 7: Schematic diagram of the simulation results of<br>
function value of the MINN composite much diatring the notestial inside the PN junction diofe under a 6.4Y Figure 5. Schematic diagram of the changes in the loss Figure 7: Schematic diagram of the simulation results of<br>function value of the MDNN composite model during the potential haste the PN junction dode. In the legend of Tigure 5: Schematic diagram of the changes in the loss Figure 7: Schematic diagram of the simulation results of material control diagram of the SHOM composite medical and is determined above can be seen in Figure 3. The se Figure 5: Schematic diagram of the changes in the loss<br>
Figure 7: Schematic diagram of the simulation results of<br>
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F simulation of the PV junction disole under a 0.4V forward bias. 6 and Figure 7, e0 and D frepresent efectrom concentration<br>
interval incredict and Equivalent and hole concentration, respectively; the solid line (S)<br>spatia Here, n-loss and p-loss represent the retrovaind function and hole concernation, respectively, the calib line (S)<br>Important the electron and hole spatial distribution outputs from<br>
Terestent the results output by Senturus Similar to training other neural network models, the MDNN **The value at the end of the legend indicates the applied bias<br>
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data.





voltage.

Figure 7: Schematic diagram of the simulation results of<br>potential inside the PN junction diode. In the legend of Figure<br>6 and Figure 7, eD and hD represent electron concentration<br>and hole concentration, respectively; the Figure 7: Schematic diagram of the simulation results of<br>potential inside the PN junction diode. In the legend of Figure<br>default and Hegure 7, cp and hD represent electron concentration<br>and hole concentration, respectivel Figure 7: Schematic diagram of the simulation results of<br>potential inside the PN junction diode. In the legend of Figure<br>6 and Figure 7, eD and hD represent electron concentration<br>6 and Heigene 6 and Eucentration, respect Figure 7: Schematic diagram of the simulation results of<br>
Equive 7: Schematic diagram of the simulation results of<br>
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Figure 7: Schematic diagram of the simulation results of<br>
potential inside the PN junction diode. In the legend of Figure<br>
and hele concentration, respectively; the solid line (S)<br>
represents the results output by Sent **Example 18**<br> **EXECAUSE TORE <br>
<b>EXECAUS** Expansively, and the Minima of the simulation results of potential inside the PN junction diode. In the legend of Figure 6 and Figure 7, eD and hD represent electron concentration and hole concentration, respectively; the Figure 7: Schematic diagram of the simulation results of<br>potential inside the PN junction diode. In the legend of Figure<br>of and Figure 7, eD and hD represent electron concentration<br>and hole concentration, respectively; th Figure 7: Schematic diagram of the simulation results of potential inside the PN junction diode. In the legend of Figure 6 and Figure 7, eD and hD represent electron concentration respectively; the solid line (S) end is c Figure 1. Sommarce unigrial in on the simulation reader<br>potential inside the PN junction diode. In the legend of Figure<br>6 and Figure 7, eD and hD represent electron concentration<br>and hote concentration, respectively; the potential insiste the r's planetal one is the same of respectively; the solid line (S) and Figure 7, eD and Ib represent electron concentration<br>and hole concentration, respectively; the solid line (S)<br>represents the resul of and trigue 1, the mastable the results outer that the hidden concentration, respectively; the solid line (S) represents the results output by the MDNN model.<br>The value at the end of the legend indicates the applied bia and not concentrations, respectively, are some and not concentration, respectively. The dished line (T) represents the results output by the MDNN model.<br>The value at the end of the legend indicates the applied bias voltage represents in treating with the MDMN model.<br>The (T) represents the results output by the MDNN model.<br>The value at the end of the legend indicates the applied bias<br>voltage.<br>The value at the end of the legend indicates the a The value at the end of the legend indicates the applied bias<br>The value at the end of the legend indicates the applied bias<br>voltage.<br>3 NUMERICAL RESULTS<br>To verify the effectiveness of the machine learning simulation<br>metho **The Value Consists of the coordinates of the method in the coordinates of the method and proposed above, the simulation result of a method proposed above, the simulation result of a method proposed above, the simulation 3 NUMERICAL RESULTS**<br>To verify the effectiveness of the machine learning simulation<br>method proposed above, the simulation result of a<br>one-dimensional graded PN junction diode will be presented as an<br>example. This PN junct **3 NUMERICAL RESULTS**<br>To verify the effectiveness of the machine learning simulation method proposed above, the simulation result of a one-dimensional graded PN junction diode will be presented as an example. This PN junc

DAC'24, June 23–27, 2024, San Francisco, CA, USA Zifei Cai, et al.<br>
code was compiled and run in the PyTorch environment of<br>
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DAC<sup>224</sup>, June 23-27, 2024, San Francisco, CA, USA *Tairca* can be PyTorch environment of **ACKNOWLEDGMENTS** Pycharm. The changes in the loss function value of the MDNN This work is supported in part by the National Natura DAC24, June 23-27, 2024, San Francisco, CA, USA [2161] ACCRIVITY COMENTIFY COMENTIFY (Call et al. et a DAC24, Jame 23-27, 2024, San Francisco, CA, USA Example 12. The search of the MINNY This work is supported in part by the National Natural Science was compiled and run in the PyTorch environment of This work is supported DAC24, June 23-27, 2024, San Francisco, CA, USA Zifei Cai, et al.<br>
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This work is supported in Part by the situation Nin exale was compiled and run in the PyToreh environment of<br>
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Miss. conditions is shown in Figure 5, the stentegy of alternately and the Bribi bias conditions is shown in Figure 6 and Figure 7.<br>
As can be observed from Figure 5, the stategy of alternately under grants 2023UCY/042 and 2019kVyXJIS048,<br>
As can be observed for the introduction of a result of the Sub As can be observed from Figure 5, the strategy of alternately<br>
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improvement in the accuracy of the monetal column coupl Lematics in the television of the best between the computer of the experimental in the computer of the computer o mpidly reduced to an extremely low level. From Figure 6 and<br>
IF  $\alpha$ , the interesting Neutron (Figure 1). We also the combined Rom of the compile in the combined MDN model in the combined MDN model in the combined MDN mod **Figure 7.** it can be clearly seen that the results change in the consistent with the consistent mathematic consistent mathematic intervents and the simulation results of the mathematic intervents and the consistent mathe machine learning and interest in the spectra of the step in the spectra of the need for any step in the need for any step in the smallest comparison of the mathematical comparison of the mathematical for the first time. T simulation couling of the transition accuracy of the method in the simulation accuracy and  $V$ . We<br>show the simulation couling the simulation of the simulation accuracy of the simulation accuracy in the simulation accurac

simulations.

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Somethed model of the Prince of Gaussian (Equation (1)) and Equation (13) are<br>
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### ACKNOWLEDGMENTS

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Figure 5. The composite model dur Zifei Cai, et al.<br> **ACKNOWLEDGMENTS**<br>
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