TCAD modeling aided by Machine Learning

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Research Question

What are the potential methodologies to accelerate TCAD simulation while preserving accuracy?

Background

- Technology for Computer-Aided Design (TCAD) uses finite element methods (FEMs) to numerically solve for a system of partial differential equations (PDEs).
- Multi-layer perceptron (MLP) uses hidden layers with various activation functions to learn data.
- Photoconductive Semiconductor Switch (PCSS) is an optoelectronic device which leverages a laser input source over leaky metal gate electrodes [1].
- DTCO framework shown below relies on TCAD in early process node development.

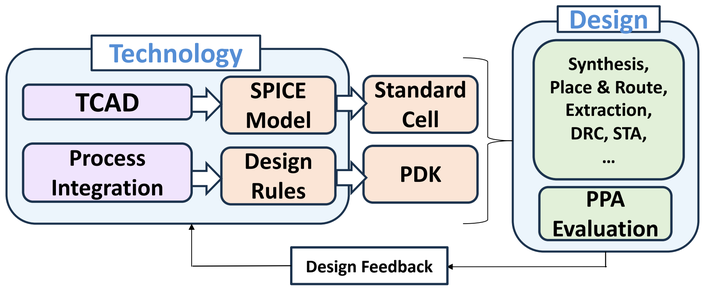

Figure 1: General design-technology co-optimization (DTCO) flow for new devices

Methodologies

- GaAs PCSS device is solved self-consistently coupling the Poisson's equation with the electron and hole equations.
- Use multi-layer perceptron model with TCAD simulated data to predict output parameters.

TCAD

Device Definition

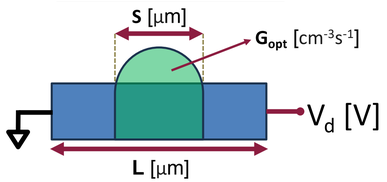

Figure 2: PCSS Device Structure [1]

Example Output Characteristic:
- Electron/hole density [cm^{-3}] at drain terminal.

Pre-processing

Training, validation, and test set with fully connected layers.

Optimizer: Adam
Learning rate: $1e^{-4}$

$$MSE = \frac{1}{n}\sum(\overline{y_i} - y_i)^2$$

MLP DNN

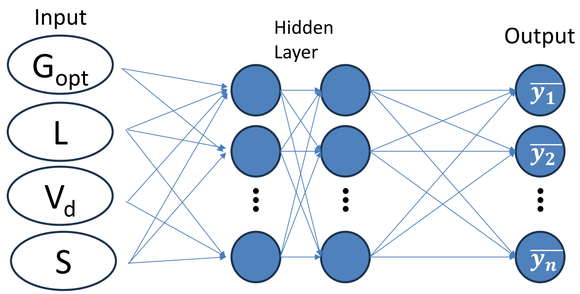

Figure 3: Workflow to train DNN model for TCAD

Goal

- Use deep learning network as an alternative for rapid convergency in PDE solutions.
- Describe the *output* characteristics of a PCSS device based on *input* design parameters using the trained DLP DNN model.
- Predict device characteristics with minimal error and quick convergence compared to TCAD runtime.
- Provide feedback efficiently for PCSS device optimization (S, Gopt, Vd, L).

Future Works

- Further train the MLP model with TCAD data using different device structures.
- Use conditional generative adversarial network (cGAN) optimize input parameters for inverse learning and data augmentation.

Figure 4: Training cGAN for optimized TCAD inputs and data augmentation.

[1] K. Dowling et al., "Pulse Compression Photoconductive Switching Using Negative Differential Mobility," in IEEE Transactions on Electron Devices, vol. 69, no. 2, pp. 590-596, Feb. 2022, doi: 10.1109/TED.2021.3136500.
[2] T. Jahan et al., 'Deep learning-driven forward and inverse design of nanophotonic nanohole arrays: streamlining design for tailored optical functionalities and enhancing accessibility', Nanoscale, vol. 16, pp. 16641–16651, 2024.

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