Machine Learning Augmented Simulation platform for semiconductor devices

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ELECTRONICS AND ELECTRICAL COMMUNICATIONS ENGINEERING

(Visual Information Processing and Embedded Systems)

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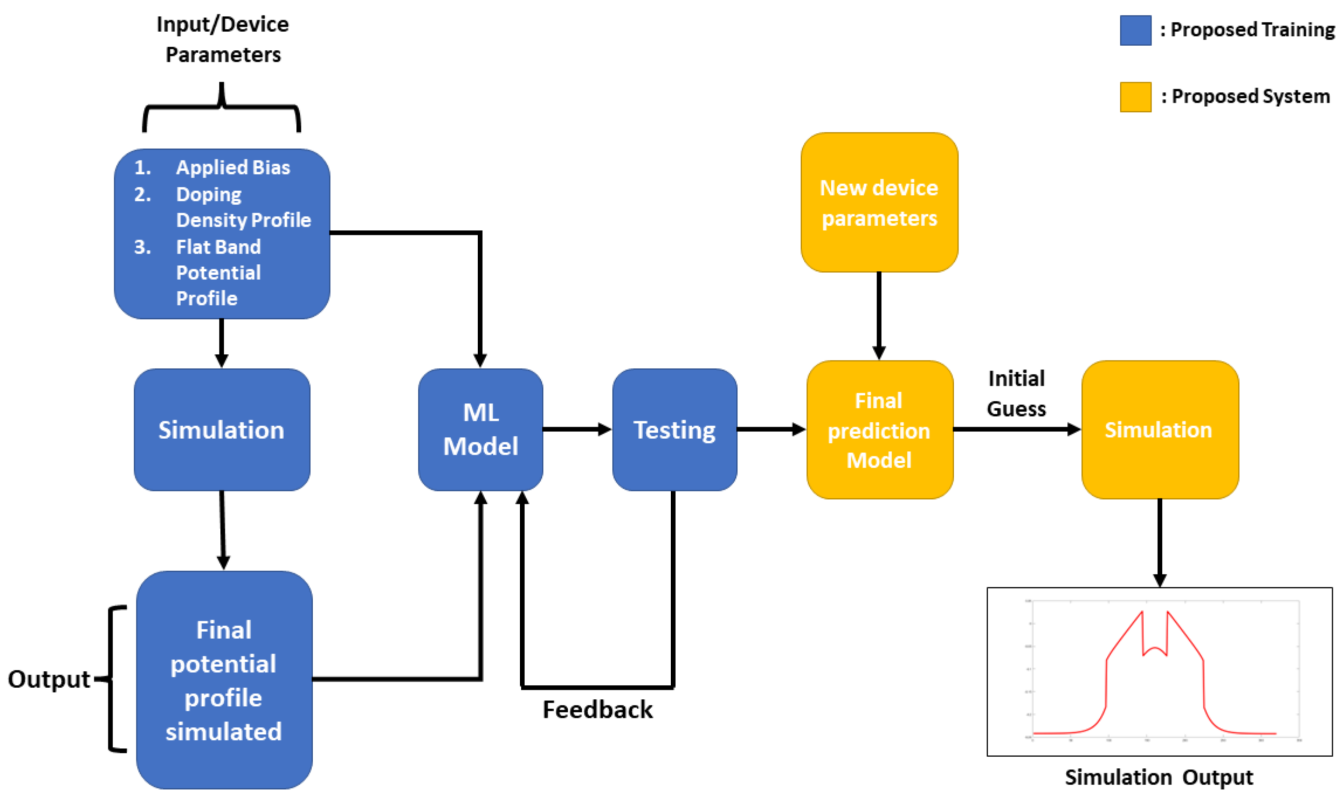
The project's goal is to develop a machine learning model that can predict simulation results for a multi-junction semiconductor device in the nano-meter range. This is because fully-quantum-mechanical simulation using non-equilibrium Green's function (NEGF) is computationally expensive and does not always provide reliable results. By training the machine learning model with NEGF simulation results and pre-processing the data, the model can help reduce the error between predicted and actual simulation results. This will make the NEGF computation easier and ensure accurate results for every test case.

Overview of steps involved in the process are –

1. Data Acquisition and Pre-processing
   Using a well-defined multi-junction device outline in MATLAB we use the NEGF function we populate training data for the model for various cases of bias, doping profile and flat band profiles. Data is processed to be fed into the model for training and testing.

2. Selecting, Tuning and Training a prediction model
   Different kinds of models with various hyper-parameters are trained and tested using the data from the previous step so that we can decide on the best choice of the prediction model as per accuracy.

3. Model output of new data and comparison of convergence time and result
   Output for datapoint is then predicted from the model and then fed to the NEGF simulator as initial guess data for that specific datapoint. Convergence times are then compared between default initial guess result and the one with model predicted initial guess and their output are compared for correctness.



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