SPINO: A Physics-Informed Fourier Neural Operator Surrogate for Accelerating Schrodinger-Poisson Simulation of Nanoscale Gate-All-Around Transistors

Pisupati, Aashrith (School: Nikola Tesla STEM High School)

Gate-all-around (GAA) transistors are central to the development of next-generation 2 nm-node semiconductor technologies, but their operation is strongly governed by quantum confinement, requiring solving the coupled Schrodinger–Poisson (SP) equations for accurate simulations. High-fidelity SP simulation is computationally expensive, limiting rapid device iteration. This research investigates whether integrating a Physics-Informed-Fourier-Neural-Operator (PI-FNO) into the SP self-consistent loop can enable fast and accurate GAA simulation. A three-dimensional Schrodinger–Poisson solver was developed for GAA nanosheet & nanowire cross-sections and used to generate a high-resolution dataset spanning variations in gate voltage, doping concentration, temperature, and device geometry. A PI-FNO was trained to predict electron density from electrostatic potential during the SP iteration, using additional residual losses. The trained model replaced most Schrodinger eigenvalue solves, with residual-based corrections. The hybrid solver was benchmarked against a research-grade baseline Schrodinger–Poisson solver for simulations across 120 sampled device conditions over 100 seeds. The baseline solver yielded a mean speedup of 1030%. Both approaches had 100% convergence. Mean relative integrated charge error was 0.04%, with sub-band energy levels and gate capacitance curves reproducing baseline values within 1.2% max error across the full voltage range. Overall, the hybrid model showed high agreement with governing physical equations and was significantly faster than the baseline. This approach illustrates the potential for PI-FNOs to enable rapid quantum-accurate GAA simulation, accelerating the development of next-generation semiconductor devices at the nanoscale.

Awards Won:

Fourth Award of $600