# 1D Self-Consistent Schrödinger-Poisson Solver for Modeling of Silicon-Based Nanoscale Transistors Tool

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## Motivation

- Accurate Nanoscale Modeling: Quantum effects are essential for understanding modern MOSFETs, requiring advanced modeling.
- Accessible Research Tool: A GUI-based simulator with NanoHub deployment makes quantum device analysis easier for students and researchers.

## Project Outcomes

- Developed a self-consistent 1D Schrödinger-Poisson solver to model quantum effects in nanoscale silicon devices.
- Implemented a user-friendly GUI allowing users to configure device parameters and view results interactively.
- Initiated NanoHub integration enabling broader access and future use in research and education.

## Uniqueness & Applications

- Models' quantum effects with Schrödinger-Poisson solver.
- Easy-to-use GUI for interactive simulation.
- Useful for MOS, MOSFET, and SOI analysis in research and education.

## Mathematical Model

**POISSON EQUATION**

- Governs the electrostatic potential ϕ(x) due to charge distribution ρ(x).
- Expressed as: $\frac{d^2\phi}{dx^2} = -\frac{\rho}{\epsilon}$
- Necessary for modeling charge behavior in MOS capacitors and quantum wells.

**Solution Procedure**

**a. Linearization and Discretization**

- Converts the continuous Poisson equation into a matrix-based formulation.
- Uses Finite Difference Method (FDM):
- Discretizes the spatial domain into a grid.
- Approximates second derivatives as: $\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} = -\frac{\rho_i}{\epsilon}$
- Leads to a system of linear equations in matrix form.

**b. Numerical Solution – LU Decomposition**

- The discretized Poisson equation results in a sparse linear system, solved efficiently using LU decomposition.
- Steps:

1. Factorizes the coefficient matrix A into L (lower triangular) and U (upper triangular) matrices.
2. Uses forward and backward substitution to compute ϕ(x).

- Provides a fast and stable method for solving large-scale simulations.

**SCHRODINGER EQUATION**

Shooting Method for the Schrödinger Equation

Solution Methodology

$$-\frac{\hbar^2}{2m^*}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$$

1. Guess an initial energy (E).
2. Integrate the differential equation using Runge-Kutta or Finite Difference Method.
3. Adjust E iteratively to satisfy boundary conditions (ψ = 0 at well edges).

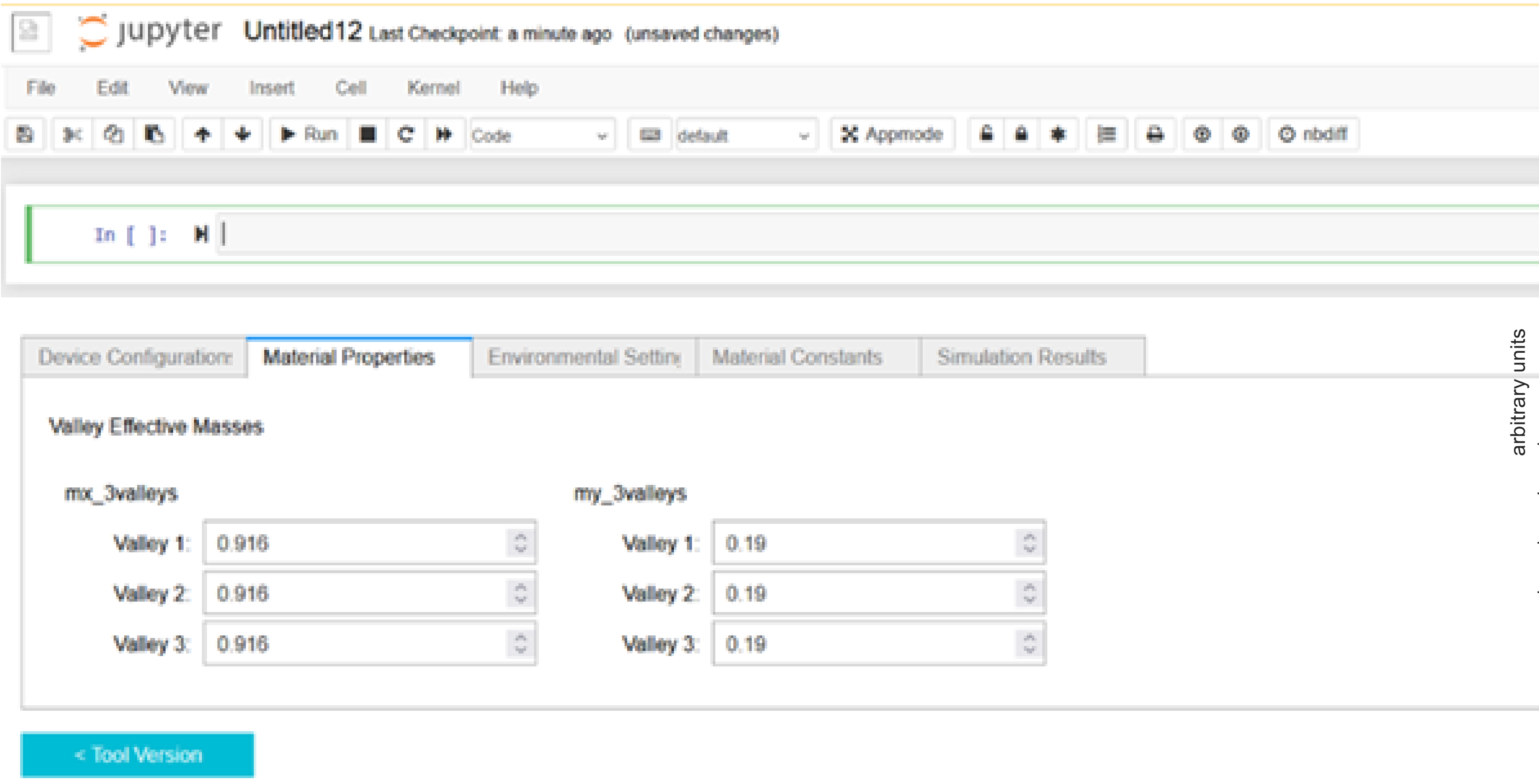
**Numerical Implementation in MATLAB**

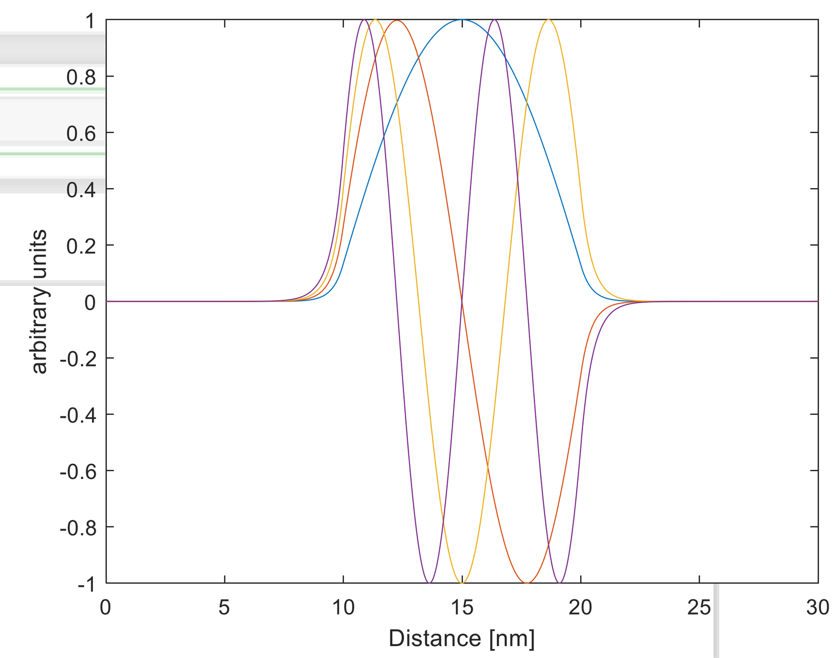
- Uses a grid-based approach for defining potential well structures.
- Implements finite difference approximation to convert Schrödinger's equation into a matrix problem.
- Solves for wavefunctions ψ(x) and energy levels E using numerical solvers.

**Finding the Eigenvalues**

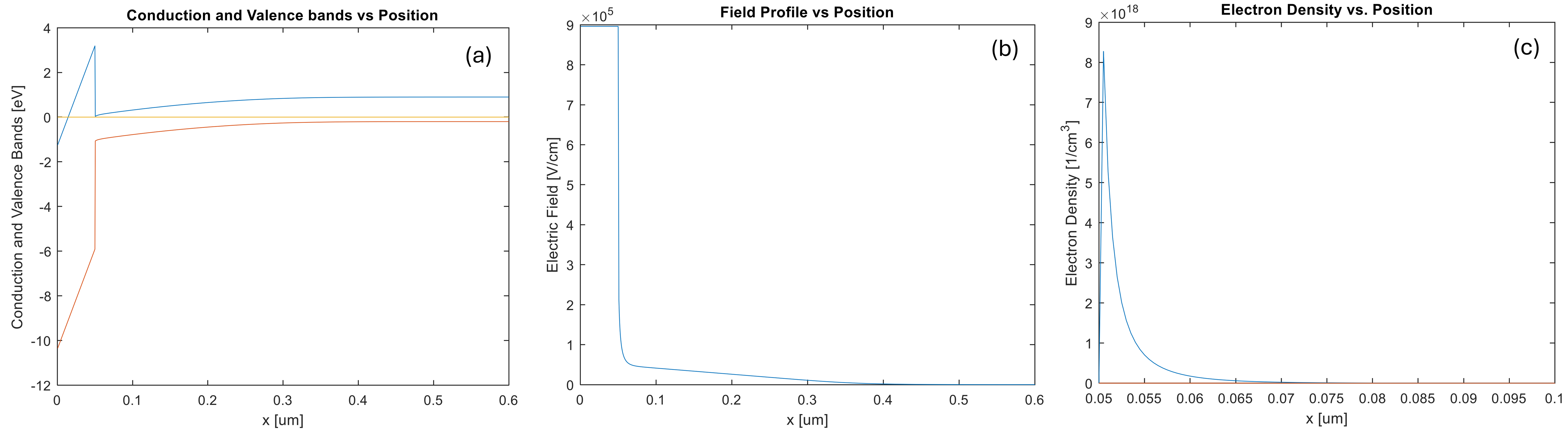
- Eigenvalues correspond to quantized energy states in the confined quantum well.
- Achieved by iterating over energy values and minimizing the residual error at the boundaries.
- The correct eigenvalue ensures a smooth wavefunction matching boundary conditions.

## Device configuration specification page of the GUI and simulation Results




Spatial variation of the lowest 4 eigenfunction




(a) Energy band diagram. (b) Variation of electric field with distance. (c) Electron density variation vs. distance