ECE 595, Section 10 Numerical Simulations Lecture 19: FEM for Electronic Transport

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February 22, 2013

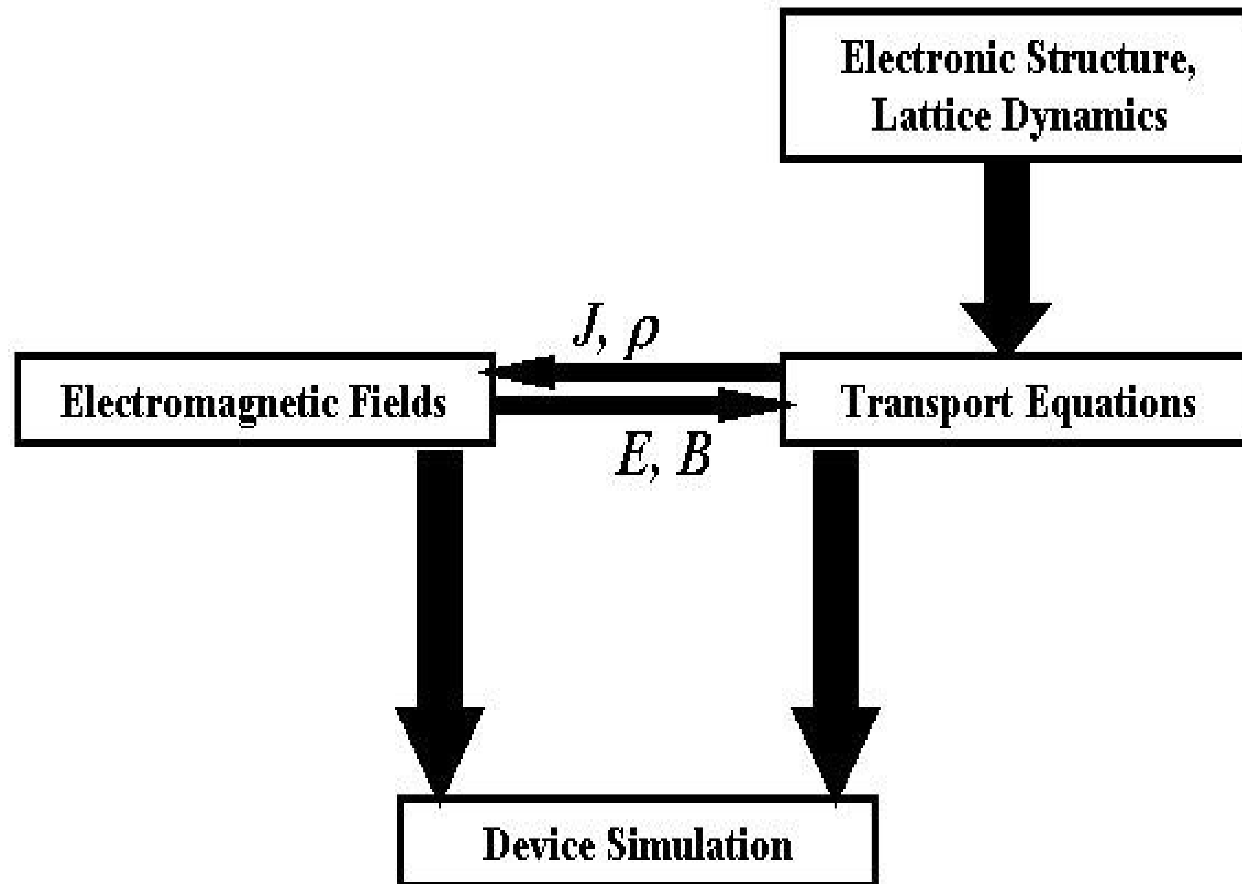
Outline

- Recap from Wednesday
- Physics-based device modeling
- Electronic transport theory
- FEM electronic transport model
- Numerical results
- Error Analysis

Recap from Wednesday

- Thermal transfer overview
  - Convection
  - Conduction
  - Radiative transfer
- FEM Modeling Approach
- Numerical Results
- Error Evaluation

Physics-Based Device Modeling



D. Vasileska and S.M. Goodnick, *Computational Electronics*, published by Morgan & Claypool , 2006.

Electronic Transport Theory

- Will assume electronic bandstructures known, and take a semiclassical approach
- Electrostatics modeled via Poissson's equation:

$$\nabla \cdot \varepsilon \nabla V = -\left(p - n + N_D^+ - N_A^- \right)$$

- Charge conservation is required:

$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \mathbf{J}_n + U_n$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot \mathbf{J}_p + U_p$$

S. Selberherr: "Analysis and Simulation of Semiconductor Devices", Springer, 1984.

Electronic Transport Theory

- Both p-type and n-type currents given by a sum of two terms:
  - Drift term, derived from Ohm's law
  - Diffusion term, derived from Second Law of Thermodynamics

$$J_n = qn(x)\mu_n E(x) + qD_n \frac{dn}{dx}$$

$$J_p = qp(x)\mu_p E(x) - qD_p \frac{dn}{dx}$$

S. Selberherr: "Analysis and Simulation of Semiconductor Devices“, Springer, 1984.

FEM Electronic Transport Model

- Much like in earlier work, will employ the following strategy:
  - Specify problem parameters, including bulk and boundary conditions
  - Construct finite-element mesh over spatial domain
  - Generate a linear algebra problem
  - Solve for key field variables: $\varphi_i\,(x,y,z,t)$

    $p\;(x,y,z,t)$

    $n\;(x,y,z,t)$

FEM Electronic Transport Model

- Regarding the grid set-up, there are several points that need to be made:
  - ✓ In critical device regions, where the charge density varies very rapidly, the mesh spacing has to be smaller than the extrinsic Debye length determined from the maximum doping concentration in that location of the device

$$L_D = \sqrt{\frac{\varepsilon k_B T}{N_{\max} e^2}}$$

  - ✓ Cartesian grid is preferred for particle-based simulations
  - ✓ It is always necessary to minimize the number of node points to achieve faster convergence
  - ✓ A regular grid (with small mesh aspect ratios) is needed for faster convergence

D. Vasileska, *EEE533 Semiconductor Device and Process Simulation* Lecture Notes, Arizona State

Poisson Solver

- The 1D Poisson equation is of the form:

$$\frac{d^2\varphi}{dx^2} = -\frac{e}{\varepsilon}(p - n + N_D - N_A)$$

$$n = n_i \exp\left(\frac{E_F - E_i}{k_B T}\right) = n_i \exp(\varphi / V_T)$$

$$p = n_i \exp\left(\frac{E_i - E_F}{k_B T}\right) = n_i \exp(-\varphi / V_T)$$

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Poisson Solver

- Perturbing potential by δ yields:

$$\frac{d^2\varphi}{dx^2} = -\frac{en_i}{\varepsilon}\left(e^{-\varphi/V_T} - e^{\varphi/V_T} + C/n_i\right) +$$

$$+\frac{en_i}{\varepsilon}\delta\left(e^{-\varphi/V_T} + e^{\varphi/V_T}\right)$$

$$\frac{d^2\varphi}{dx^2} - \frac{en_i}{\varepsilon}\left(e^{-\varphi/V_T} + e^{\varphi/V_T}\right)\varphi^{new} = -\frac{en_i}{\varepsilon}\left(e^{-\varphi/V_T} - e^{\varphi/V_T} + C/n_i\right) -$$

$$-\frac{en_i}{\varepsilon}\left(e^{-\varphi/V_T} + e^{\varphi/V_T}\right)\varphi^{old}$$

$$\delta = \varphi^{new} - \varphi^{old}$$

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Poisson Solver

- Renormalized form

$$\frac{d^2\varphi}{dx^2} = -(p - n + C) + \delta(p + n)$$

$$\frac{d^2\varphi}{dx^2} - (p + n)\varphi^{new} = -(p - n + C) - (p + n)\varphi^{old}$$

$$\delta = \varphi^{new} - \varphi^{old}$$

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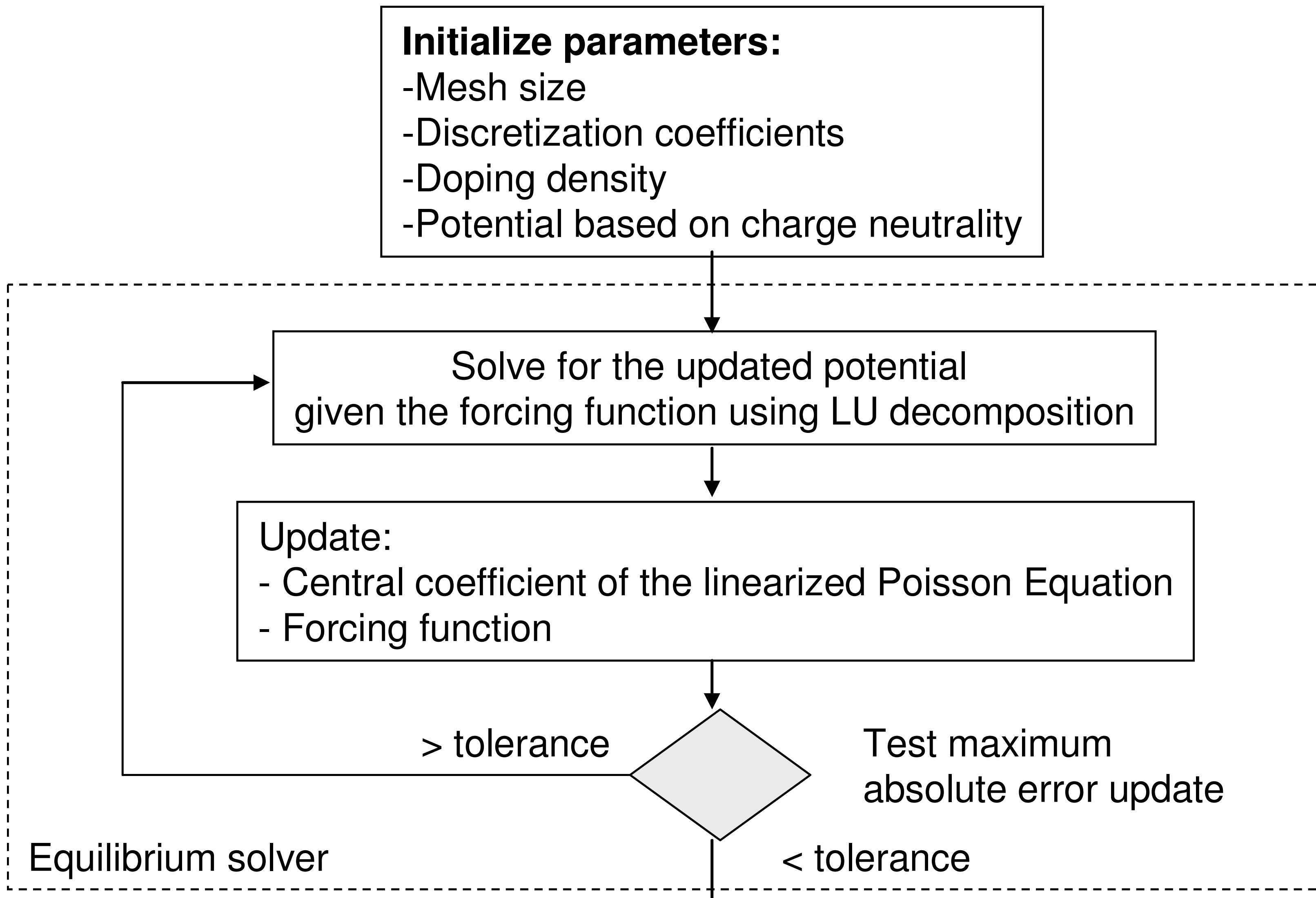
Poisson Solver



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Current Discretization

- The discretization of the continuity equation in conservative form requires the knowledge of the current densities

$$J_n(x) = en(x)\mu_n E + eD_n \nabla n$$
$$J_p(x) = ep(x)\mu_p E - eD_p \nabla p$$

on the mid-points of the mesh lines connecting neighboring grid nodes. Since solutions are available only on the grid nodes, interpolation schemes are needed to determine the solutions.

- There are two schemes that one can use:
  - (a) Linearized scheme: *V, n, p*, μ and *D* vary linearly between neighboring mesh points
  - (b) Scharfetter-Gummel scheme: electron and hole densities follow exponential variation between mesh points

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Naïve Linearization Scheme

- Within the linearized scheme, one has that

$$J_{i+1/2} = -en_{i+1/2}\mu_{i+1/2}\frac{V_{i+1}-V_i}{a_i} + eD_{i+1/2}\nabla n\big|_{i+1/2}$$

$$\frac{n_{i+1}+n_i}{2} \qquad\qquad \frac{n_{i+1}-n_i}{a_i}$$

$$J_{i+1/2} = n_{i+1}\left[-\frac{e\mu_{i+1/2}}{2}\frac{V_{i+1}-V_i}{a_i} + \frac{eD_{i+1/2}}{a_i}\right] - n_i\left[\frac{e\mu_{i+1/2}}{2}\frac{V_{i+1}-V_i}{a_i} + \frac{eD_{i+1/2}}{a_i}\right]$$

- This scheme can lead to substantial errors in regions of high electric fields and highly doped devices.

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Scharfetter-Gummel Scheme

- One solves the electron current density equation

$$J_{i+1/2} = -en\mu_{i+1/2}\frac{V_{i+1}-V_i}{a_i} + eD_{i+1/2}\frac{\partial n}{\partial x}$$
$$= -en\mu_{i+1/2}\frac{V_{i+1}-V_i}{a_i} + eD_{i+1/2}\frac{\partial n}{\partial V}\frac{\partial V}{\partial x}$$

for $n(V)$, subject to the boundary conditions

$$n(V_i) = n_i \quad \text{and} \quad n(V_{i+1}) = n_{i+1}$$

- The solution of this first-order differential equation leads to

$$n(V) = n_i[1 - g(V)] + n_{i+1}g(V), \quad g(V) = \frac{e^{(V-V_i)/Vt} - 1}{e^{(V_{i+1}-V_i)/Vt} - 1}$$
$$J_{i+1/2} = \frac{eD_{i+1/2}}{a_i}\left[n_{i+1}B\left(\frac{V_{i+1}-V_i}{Vt}\right) - n_iB\left(\frac{V_i-V_{i+1}}{Vt}\right)\right]$$
$$B(x) = \frac{x}{e^x - 1} \quad \text{is the Bernouli function}$$

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ADEPT 2.0

- Available on nanoHUB from Prof. Gray's team: https://nanohub.org/tools/adeptnpt

ADEPT 2.0 | Terminate | Keep for later

1 Simulation Option → 2 Parameter → 3 Simulate | About this tool | Questions?

Layer | Absorption | Global | Simulation

Example: Simple c-Si solar cell in light

Number of Layer: 3

Layer # 1 | Layer # 2 | Layer # 3

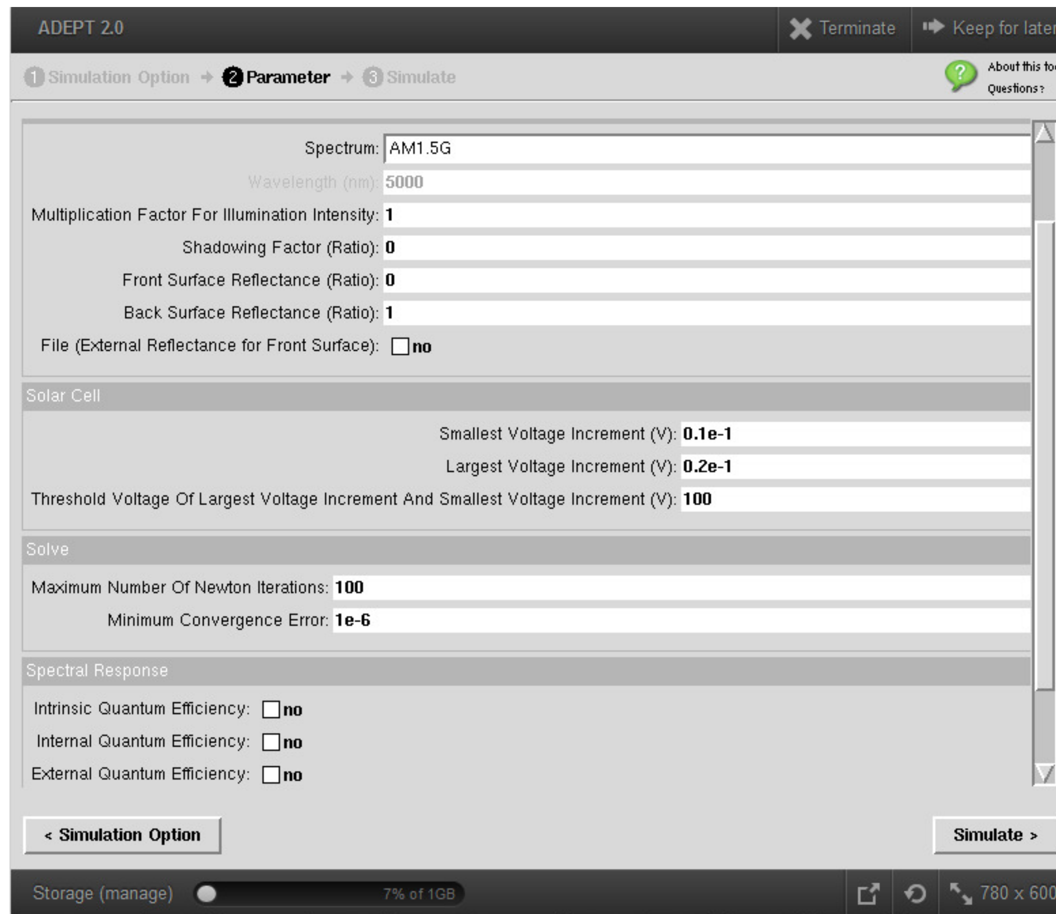
Parameter	Value
Filter Layer:	no
Layer Thickness (um):	0.3
Doping Type:	n type
Dopant Density (cm-3):	6e19
Bandgap (eV):	1.03
Electron Affinity (eV):	4.05
Dielectric Constant:	11.7
Conduction Band Effective Density Of States (cm-3):	2.82e19
Valence Band Effective Density Of States (cm-3):	2.65e19
Electron Mobility (cm2 V-1 s-1):	80.1
Hole Mobility (cm2 V-1 s-1):	52.8
SHR Electron Lifetime (s):	33.7e-6
SHR Hole Lifetime (s):	33.7e-5
Auger Electron Recombination Coefficient (cm6 s-1):	0.28e-30
Auger Hole Recombination Coefficient (cm6 s-1):	0.099e-30

< Simulation Option | Simulate >

Storage (manage) 7% of 1GB | 780 x 600

ADEPT 2.0

- Can customize all the calculation details:



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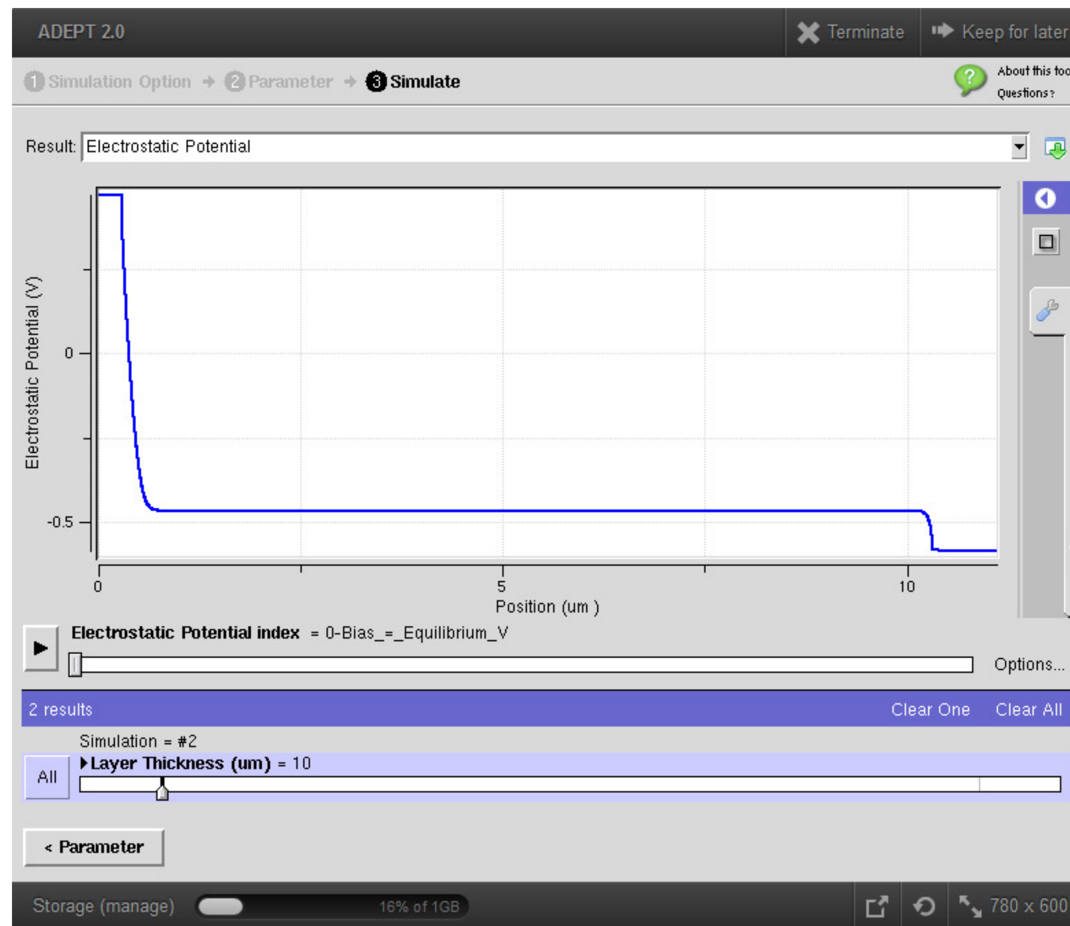
- Outputs include electrostatic (Poisson) solution:



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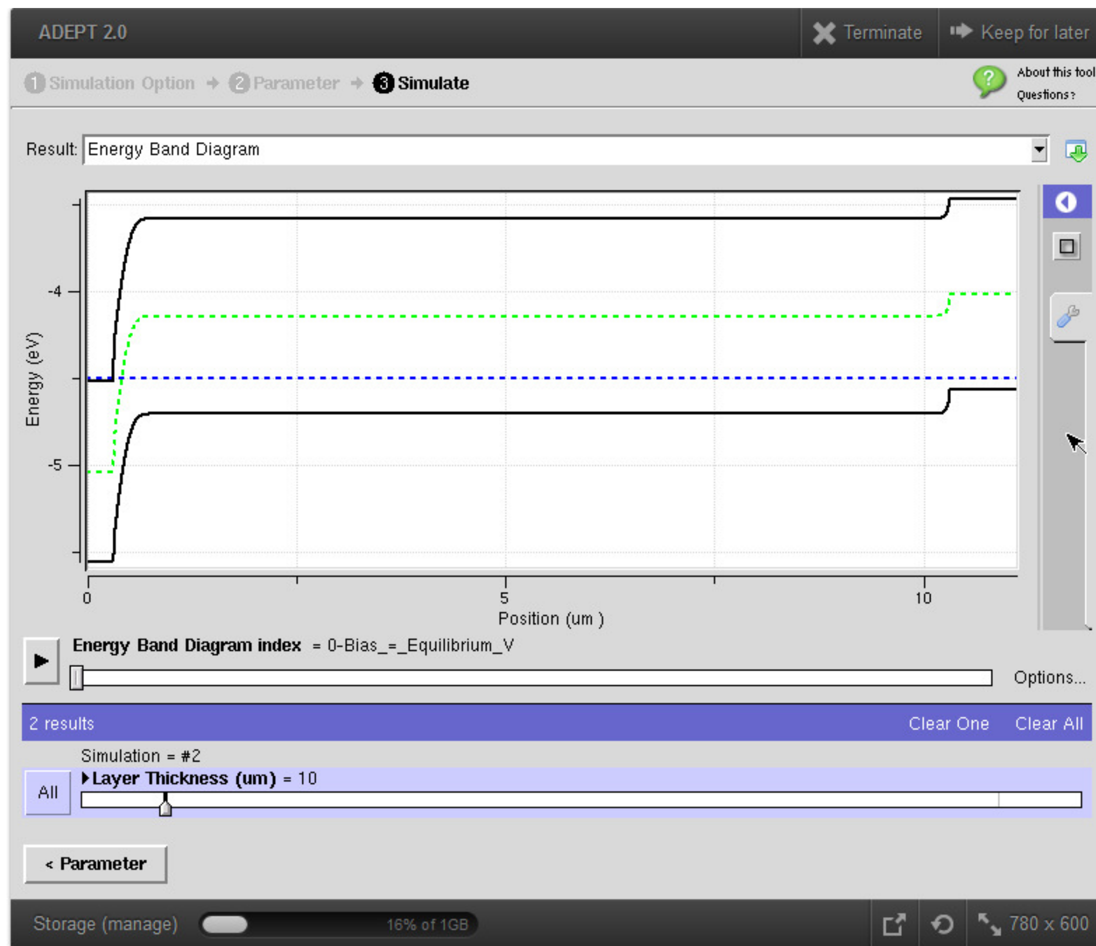
- Energy band diagram



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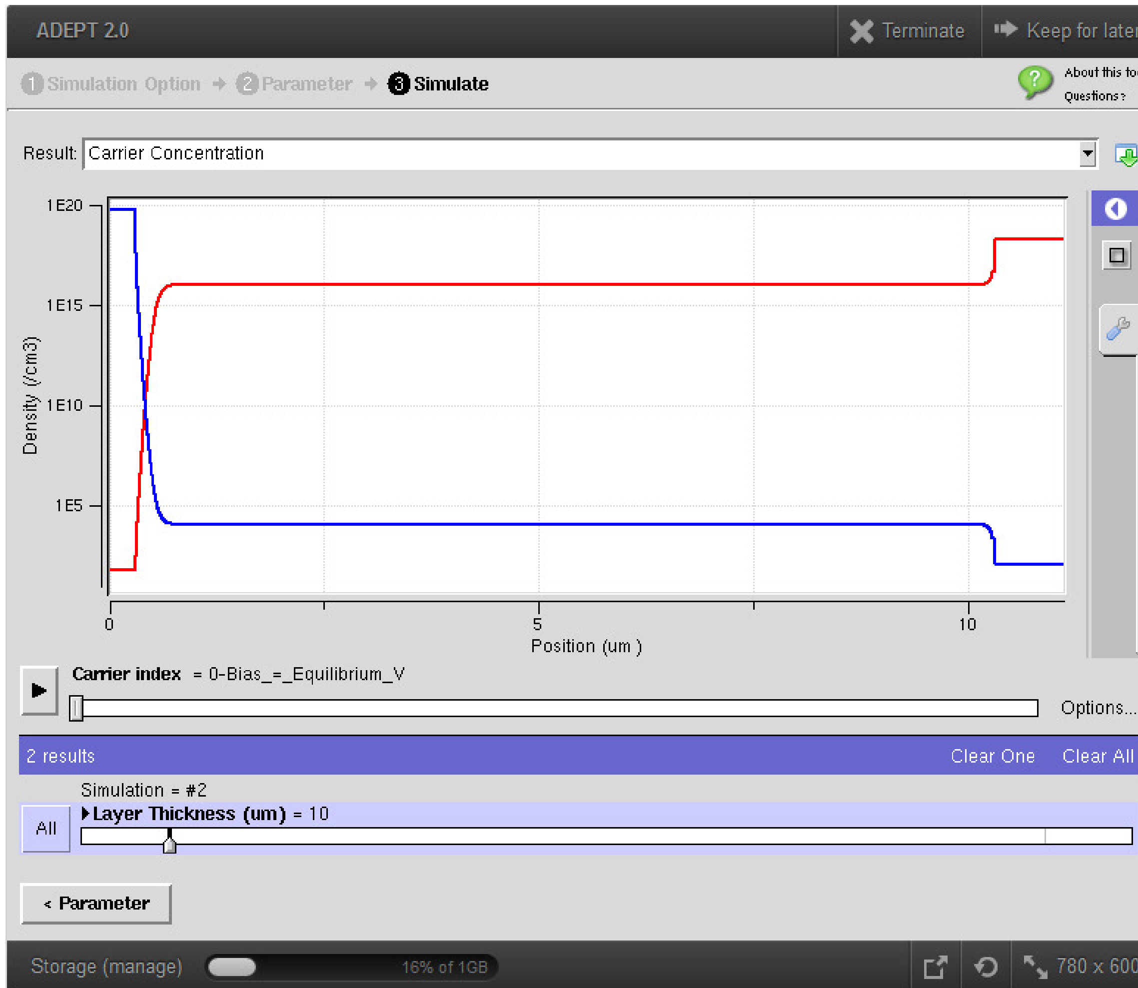
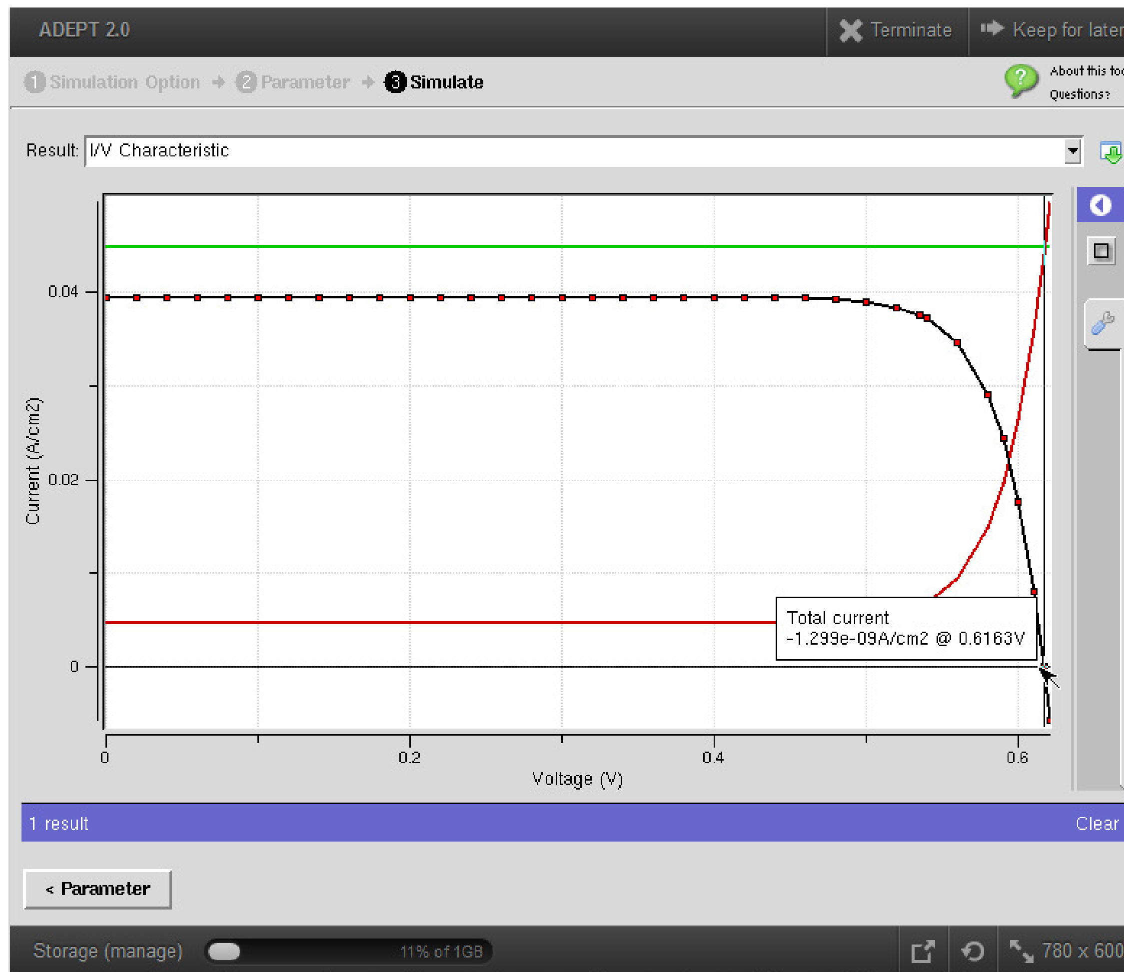
- Carrier concentrations:



ADEPT 2.0

- And finally, realistic I-V curves:



Next Class

- Is on Monday, Feb. 25
- Next time, we will cover electronic bandstructures