ECE 695
Numerical Simulations
Lecture 14: Drift-Diffusion Simulations

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Outline

- Recap of Drift-Diffusion Model
- Solar Cell Physics
- ADEPT
  - Overview
  - Input modalities and options
  - Output data and interpretation

Drift-Diffusion Model

- Electrostatics (Poisson's equation):

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

- Charge conservation:

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

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

- Current from drift & diffusion terms:

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

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

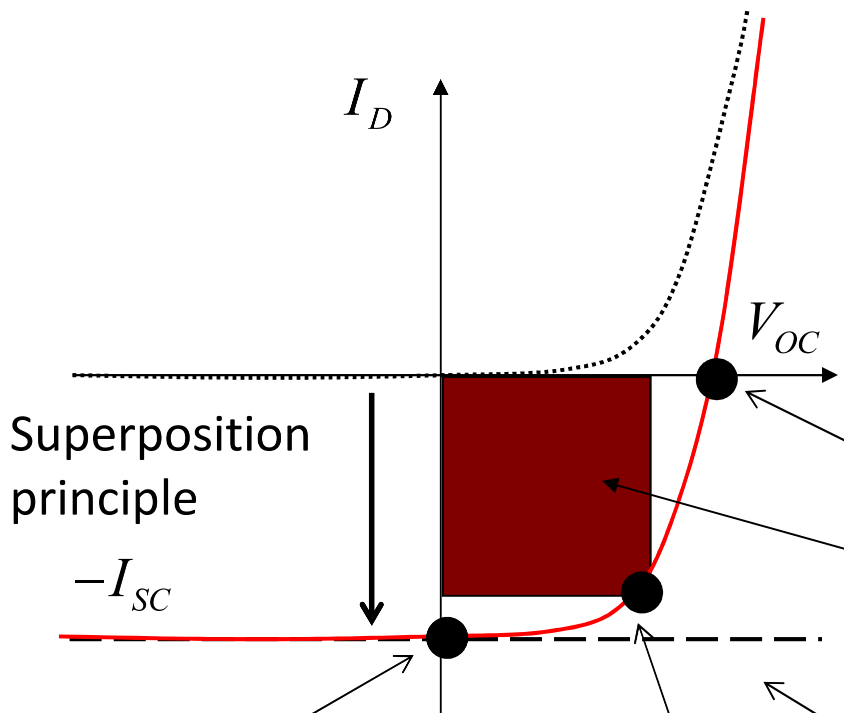
S. Selberherr: "Analysis and Simulation of Semiconductor Devices“, Springer, 1984.

Solar Cells: Ideal IV Characteristics

$$I_D = I_0\left(e^{qV_D/k_BT} - 1\right)$$

$$I_{TOT} = I_0\left(e^{qV_D/k_BT} - 1\right) - I_{SC}$$

$$\eta = \frac{P_{out}}{P_{in}} = \frac{I_{SC}V_{OC}FF}{P_{in}}$$



$$P_{out} = I_{TOT}V_{OC} = 0$$

Maximum power rectangle

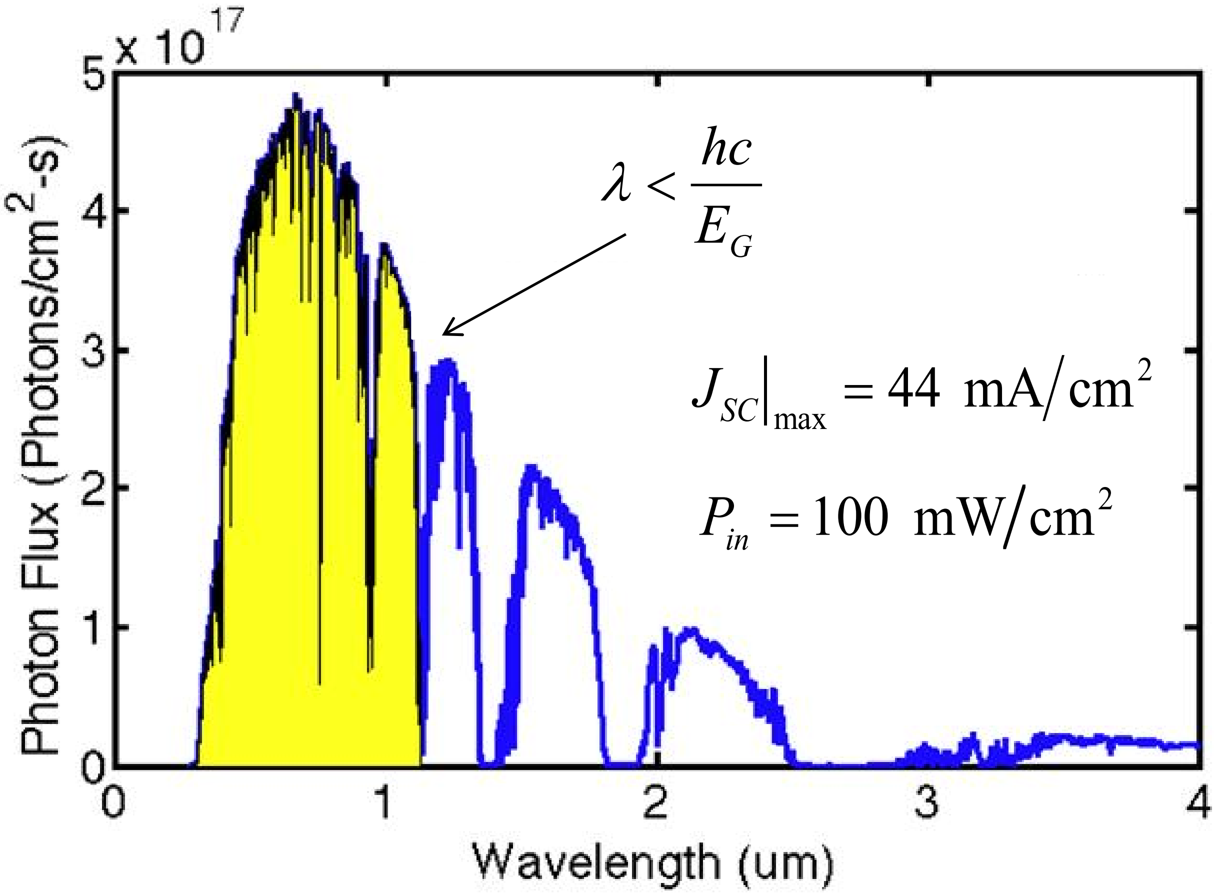
$$P_{out} = -I_{SC}V_D = 0$$

$$P_D = I_{TOT}V_D < 0$$

$$\left|P_{out}\right| = I_{mp}V_{mp} = -I_{SC}V_{OC}FF$$

Maximum Short Circuit Current

Example: Silicon E_g = 1.1eV. Only photons with a wavelength < 1.12 μm will be absorbed.



solar spectrum (AM1.5G)

Open-circuit Voltage and Efficiency

$$I_{TOT} = I_0\left(e^{qV/k_BT} - 1\right) - I_{SC} \qquad V_{OC} = \frac{k_BT}{q}\ln\left(\frac{I_{SC}}{I_0}\right) \qquad \eta = \frac{P_{out}}{P_{in}} = \frac{I_{SC}V_{OC}FF}{P_{in}}$$

Example for silicon photovoltaics:

$$I_0 = 1\times 10^{-12}\ \text{A}$$

$$\eta = \frac{P_{out}}{P_{in}} = \frac{40\times 0.63\times 0.8}{100} = 0.20$$

$$I_{SC} = 0.90\times 44\times 10^{-3} = 40\ \text{mA}$$

$$V_{OC} = 0.026\ln\left(\frac{40\times 10^{-3}}{1\times 10^{-12}}\right) = 0.63$$

Increasing the Efficiency

$$\eta = \frac{P_{out}}{P_{in}} = \frac{I_{SC} V_{OC} FF}{P_{in}}$$

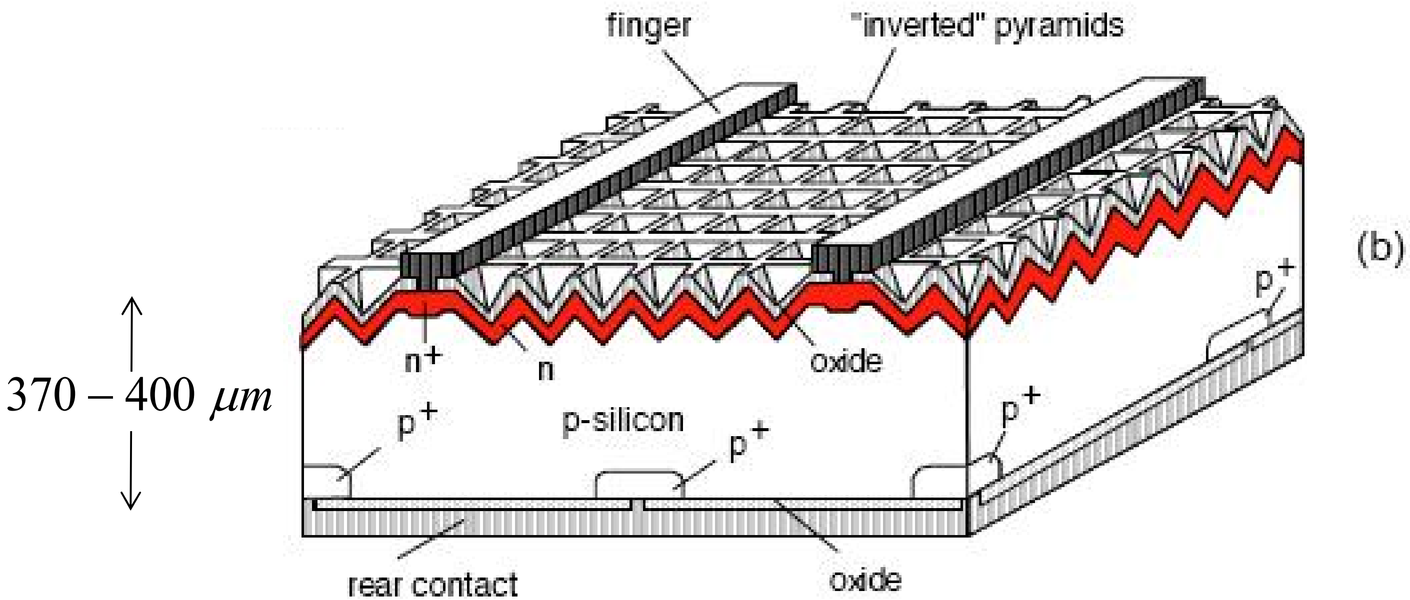
1) Increase the short circuit current from 40 towards 44

2) Increase V_{OC} (decrease I_0)

$$V_{OC} = \frac{k_B T}{q} \ln\left(\frac{I_{SC}}{I_0}\right)$$

$$I_0 = qA\left(\frac{D_n}{W_P} \frac{n_i^2}{N_A}\right)$$

Efficiency of Silicon Solar Cells (PERL Architecture)



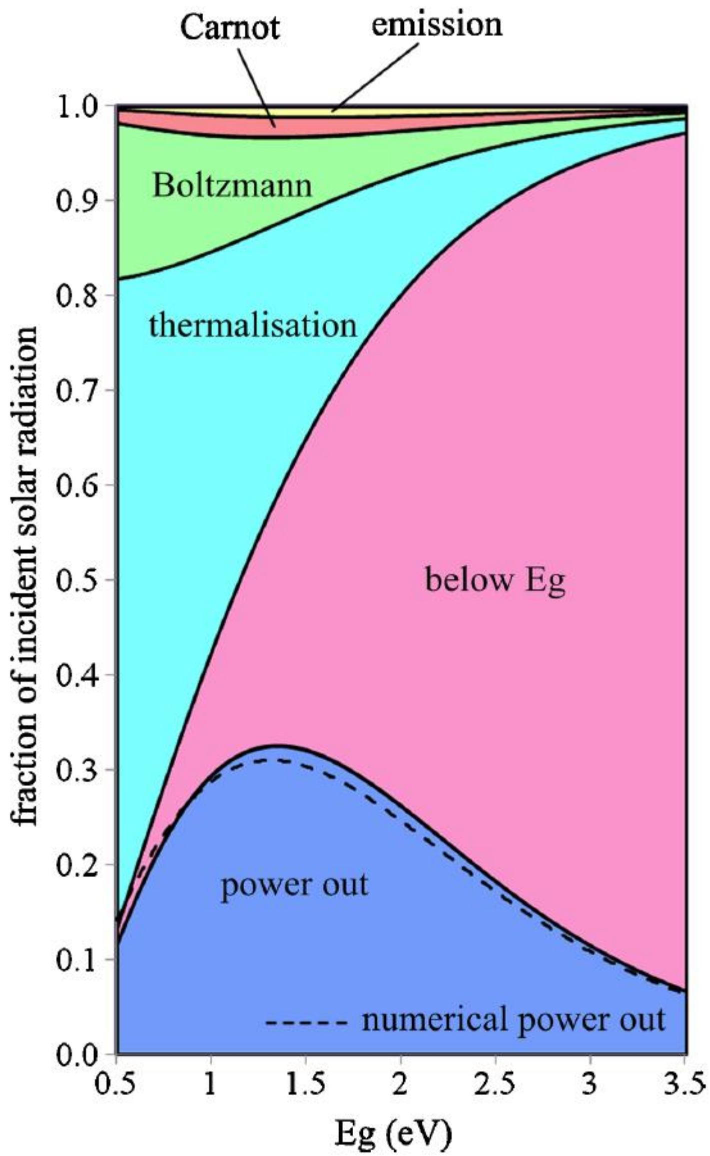
$$J_{SC} = 41.5 \text{ mA/cm}^2 \quad (94\%)$$

$$V_{OC} = 0.703 \qquad FF = 0.81$$

$$I_0 = 0.075 \times 10^{-12} \text{ A}$$

Martin Green Group UNSW – Zhao *et al*., 1998 (25% at 1 sun)

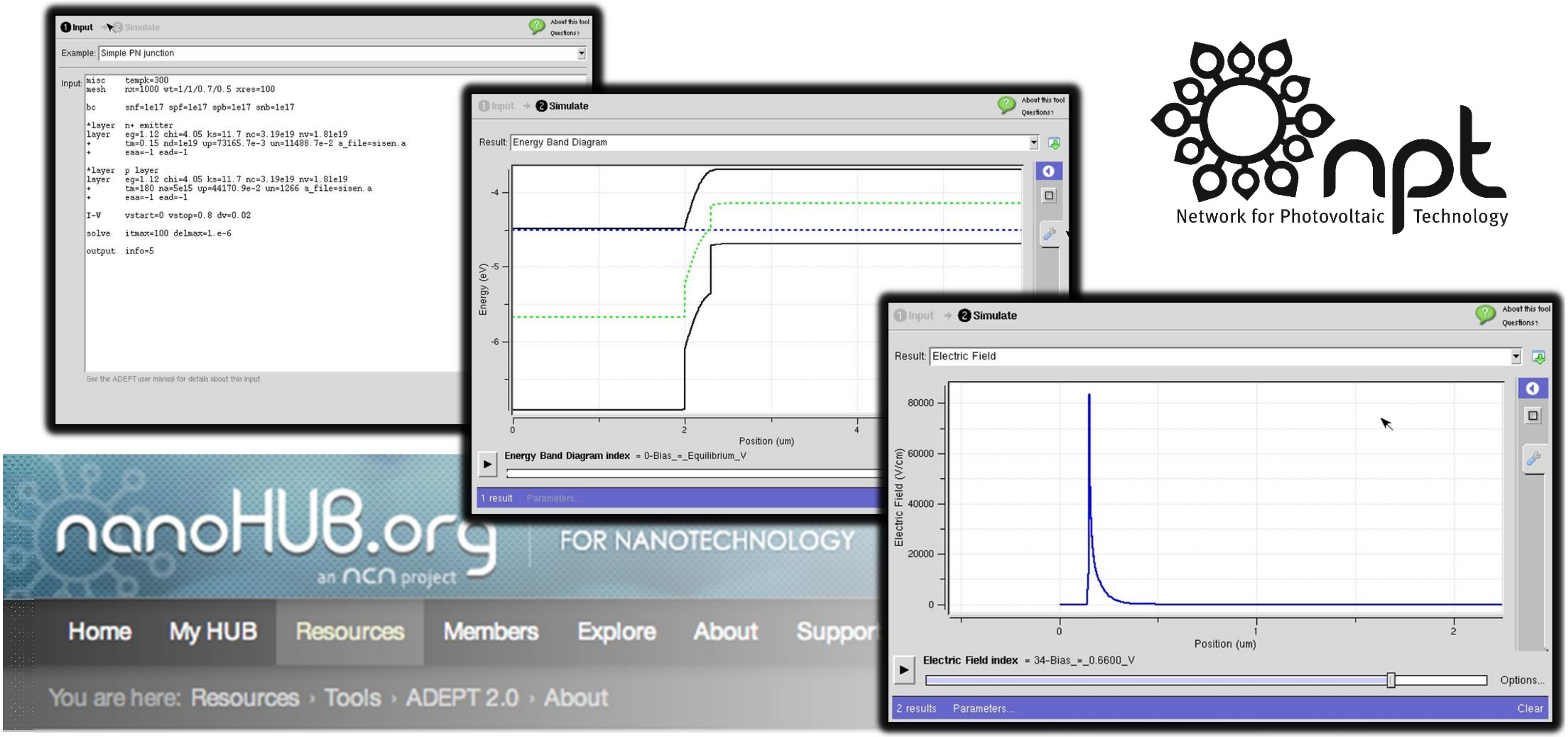
J_{SC} – V_{OC} trade-off



1) Smaller bandgaps give higher short circuit current
2) Larger bandgaps give higher open-circuit voltage
3) For the given solar spectrum, an optimum bandgap exists.

"Shockley-Queisser Limit"

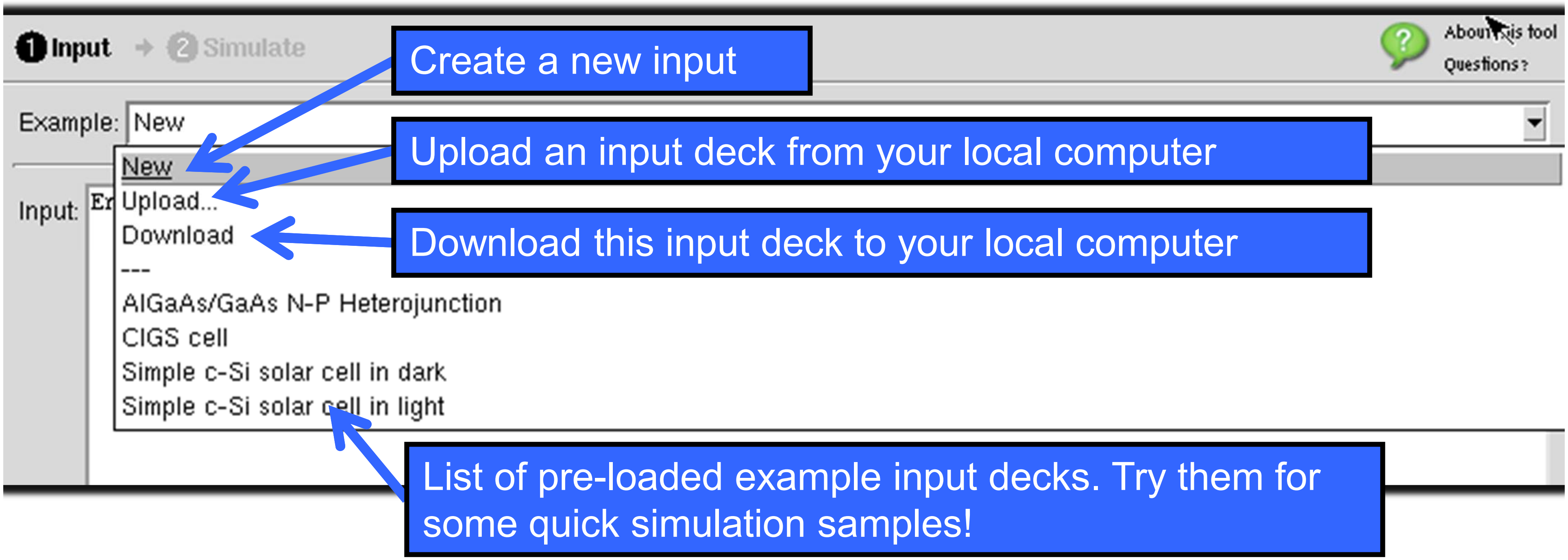
ADEPT 2



Available on nanoHUB.org via:

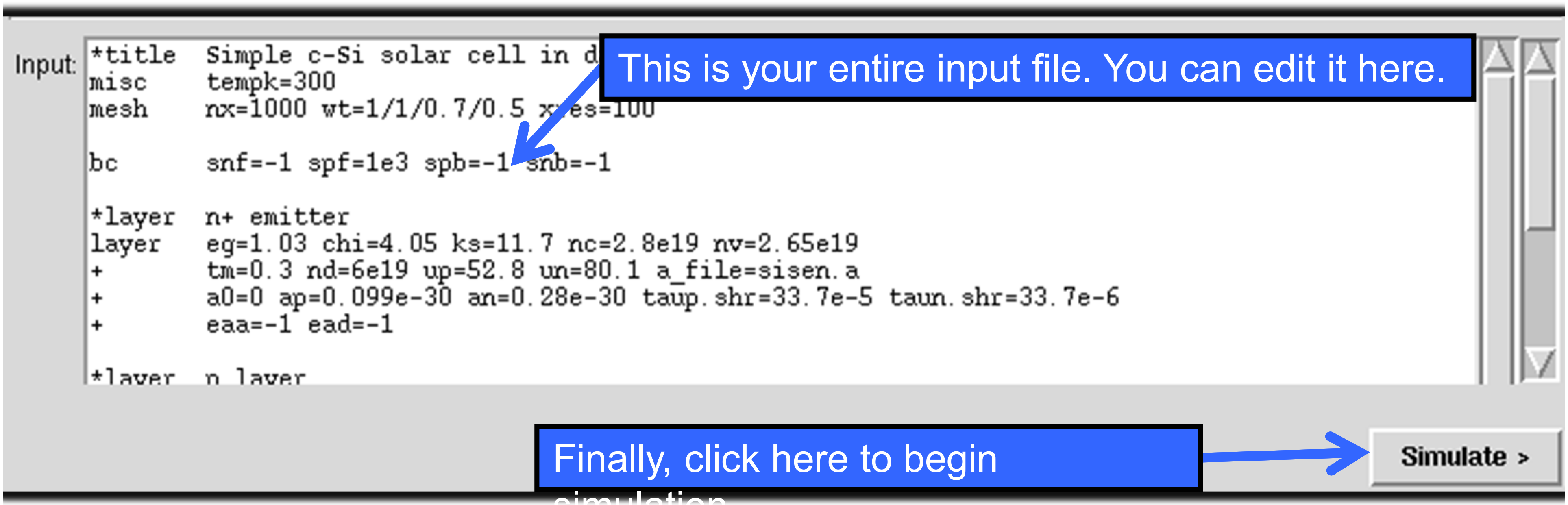
https://nanohub.org/tools/adeptnpt/

ADEPT: Input deck



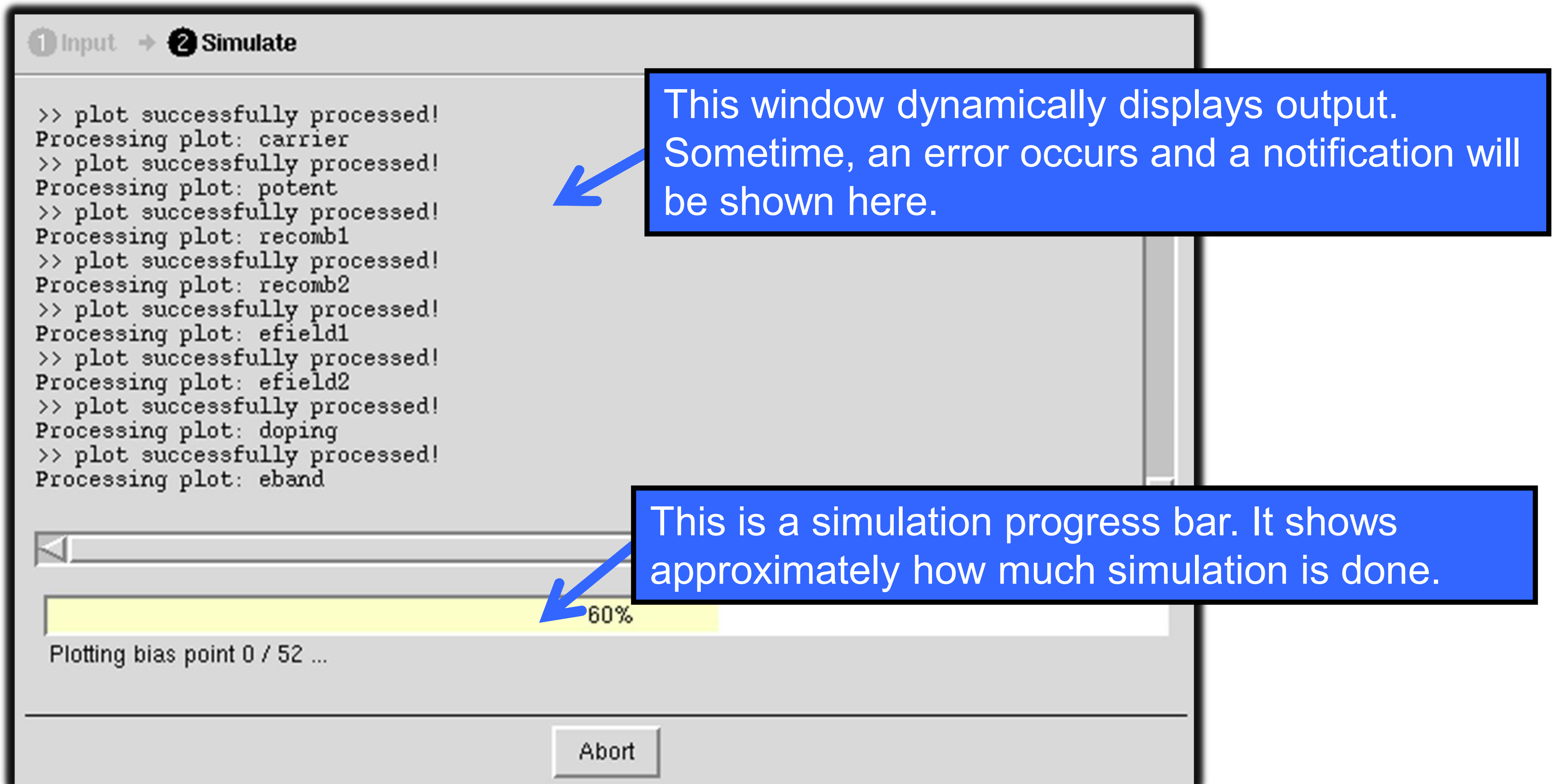
- Upon opening ADEPT 2, a blank input page will appear, awaiting your input file.
- If upload/download does not work, one reason could be “pop-up” blocking by your internet browser.

ADEPT: Running a simulation



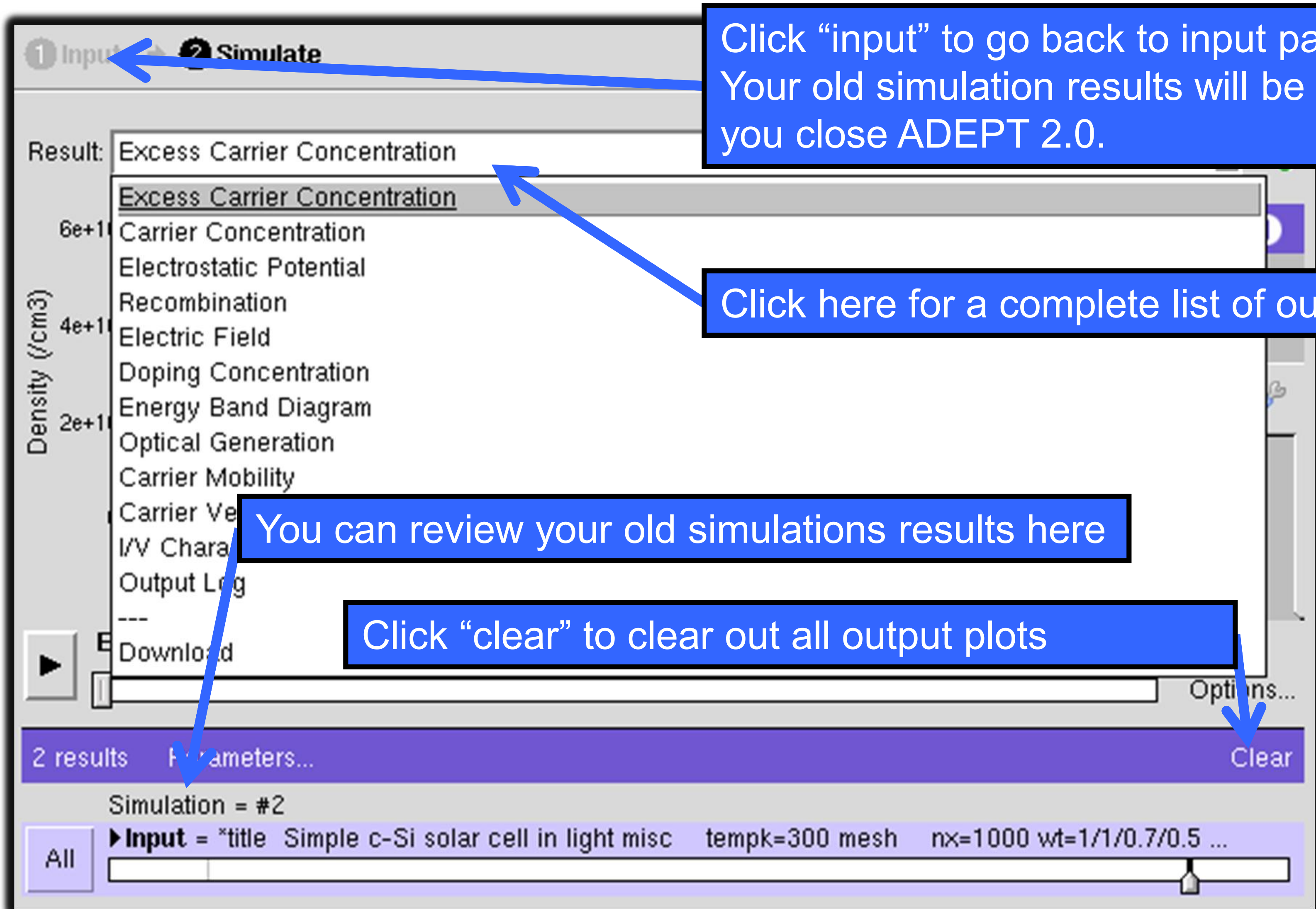
- Keep in mind that ADEPT 2 is FORTRAN 77 based. The format of certain input may cause unexpected error.
- Please refer to “ADEPT 2 User Manual” for more information regarding how to write an ADEPT input deck.

ADEPT: While simulation is running



- In ADEPT, an entire simulation consists of two parts: ADEPT simulation and PLOTA output generation.

ADEPT: Output



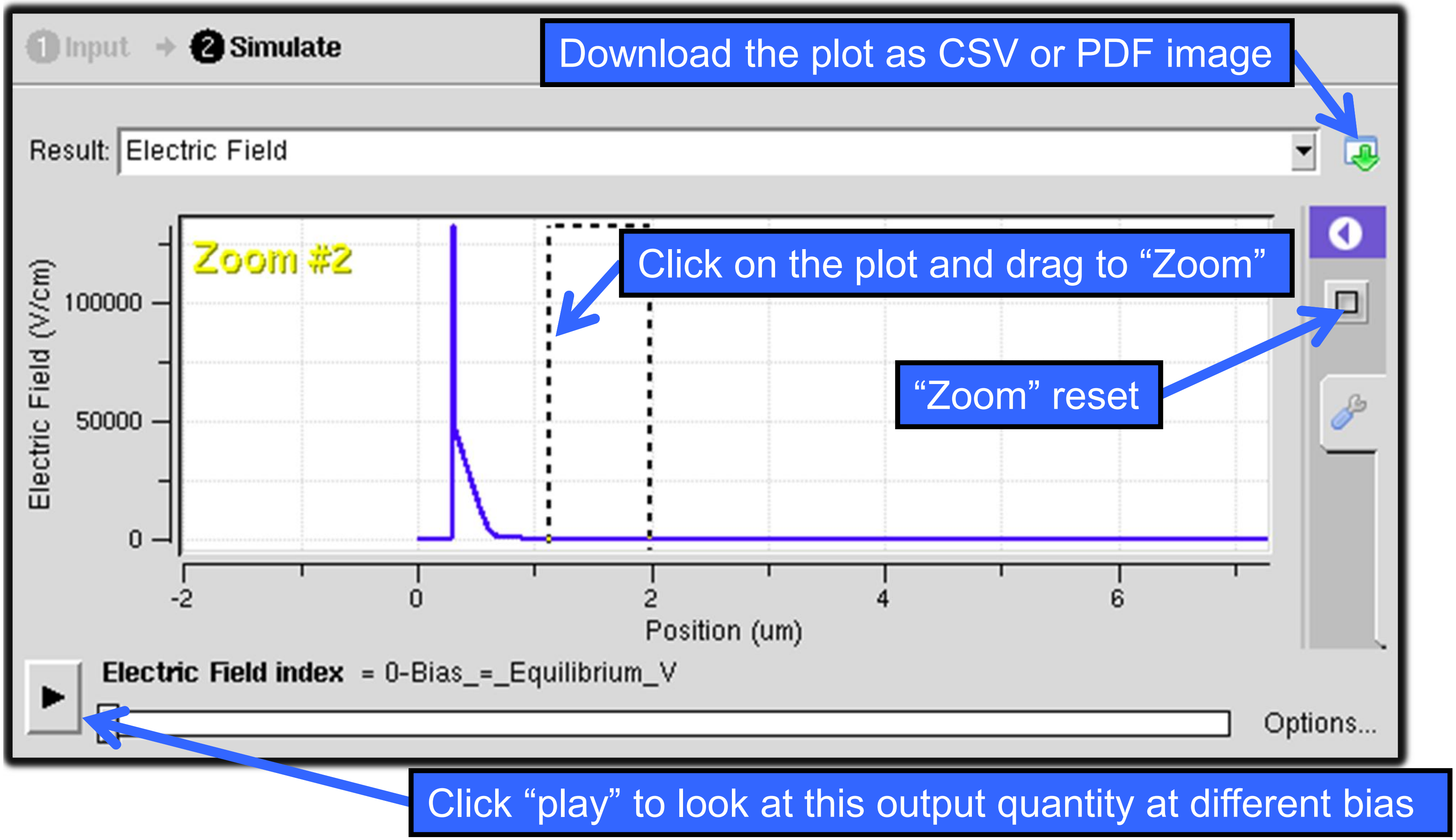
Click “input” to go back to input page. Worry not! Your old simulation results will be saved until you close ADEPT 2.0.

Click here for a complete list of output plots

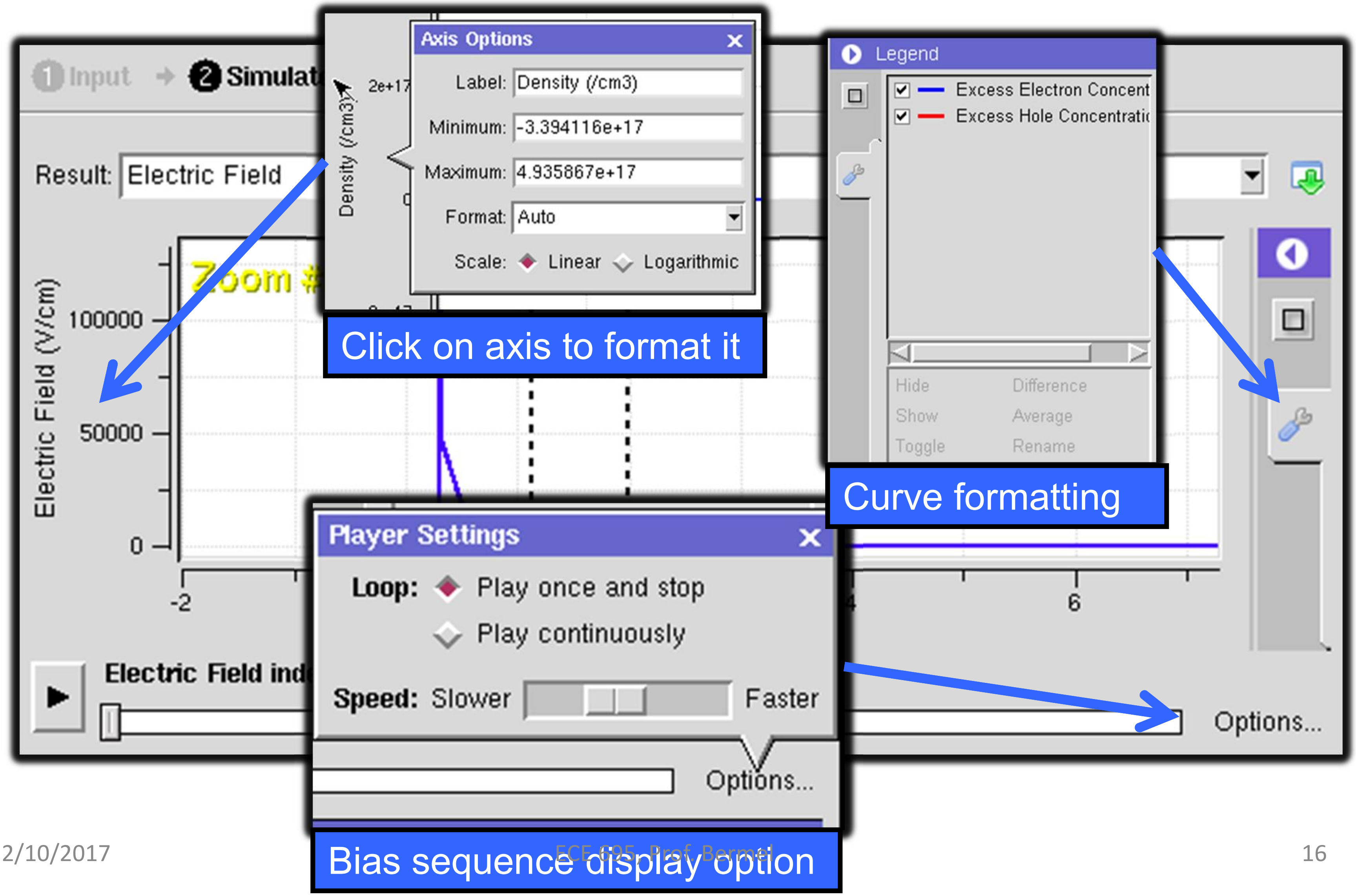
You can review your old simulations results here

Click “clear” to clear out all output plots

ADEPT: Output

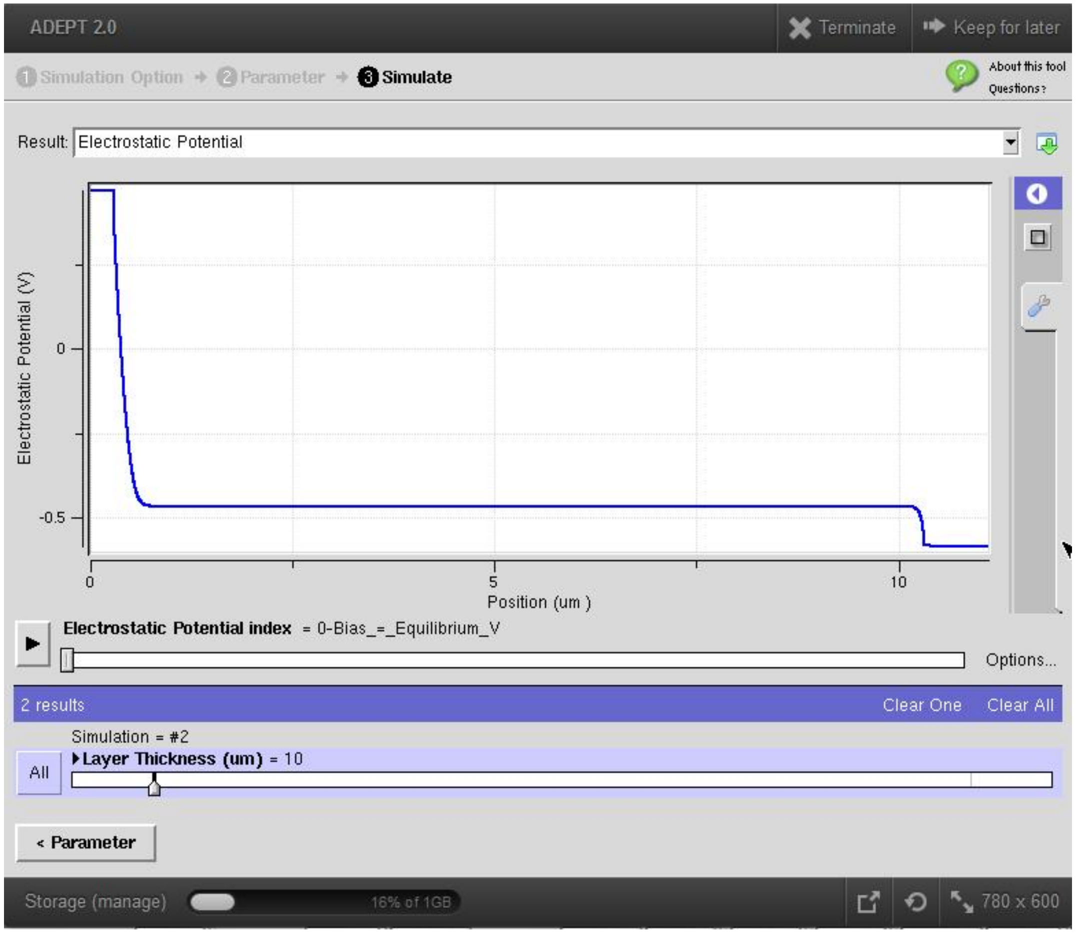


ADEPT: Output



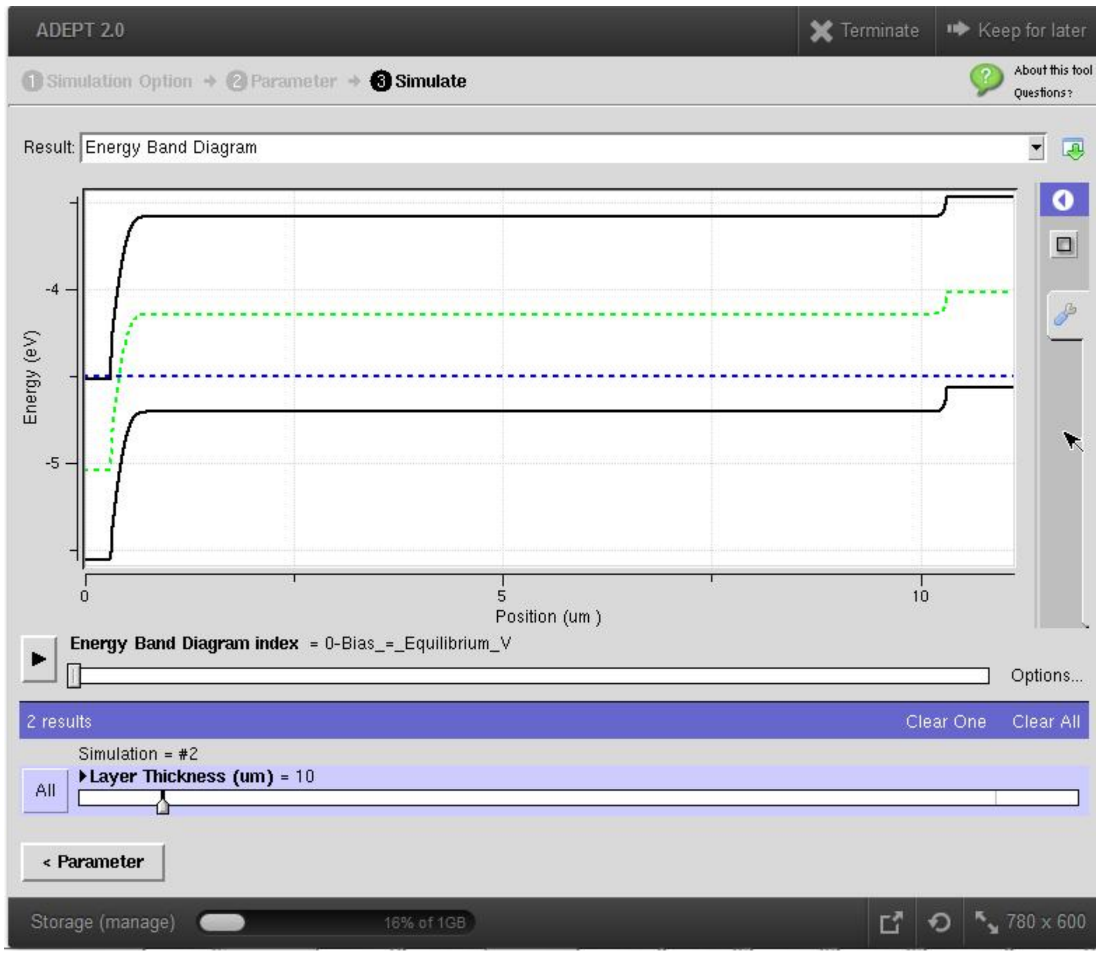
ADEPT: Output

- Outputs include electrostatic (Poisson) solution:



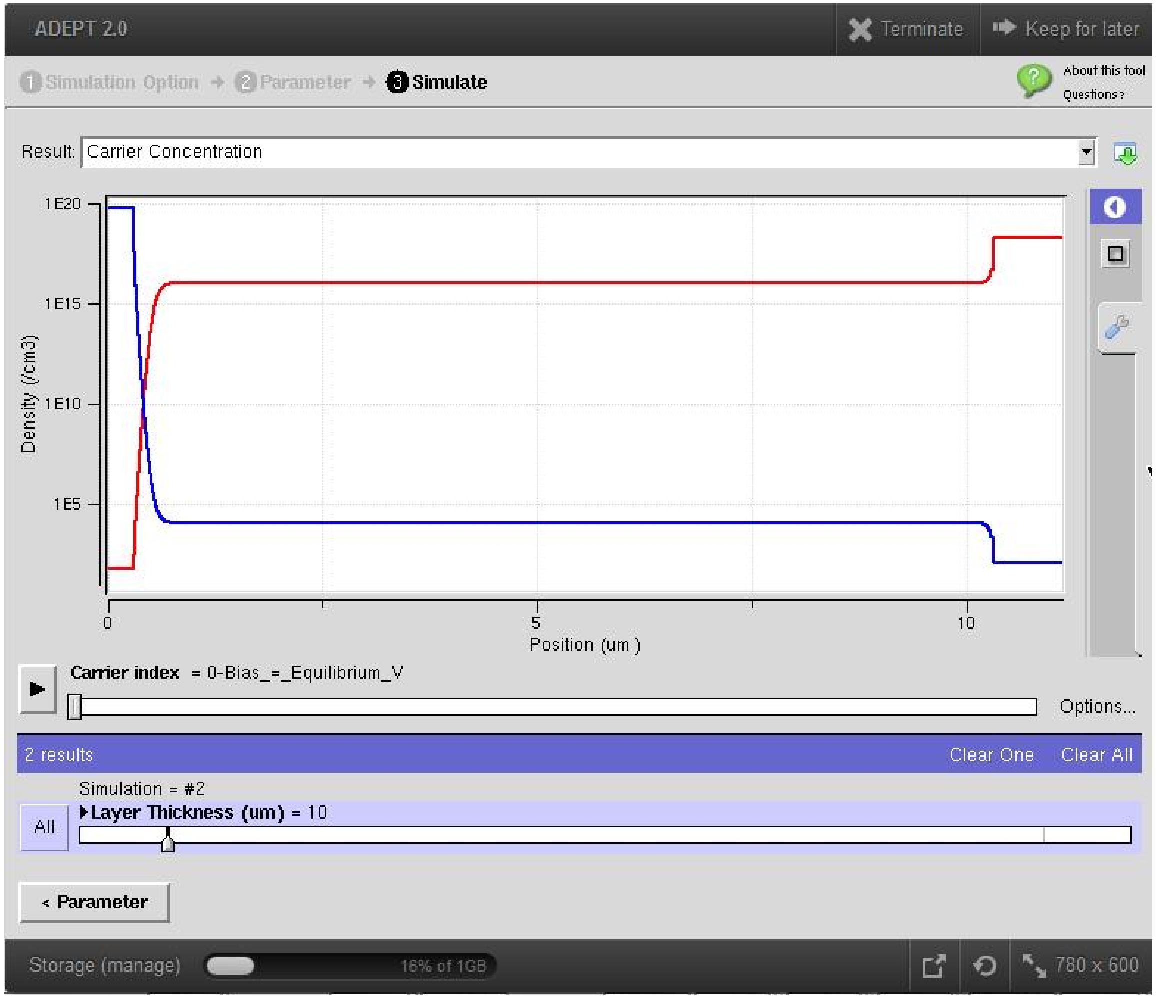
ADEPT: Output

- Energy band diagram



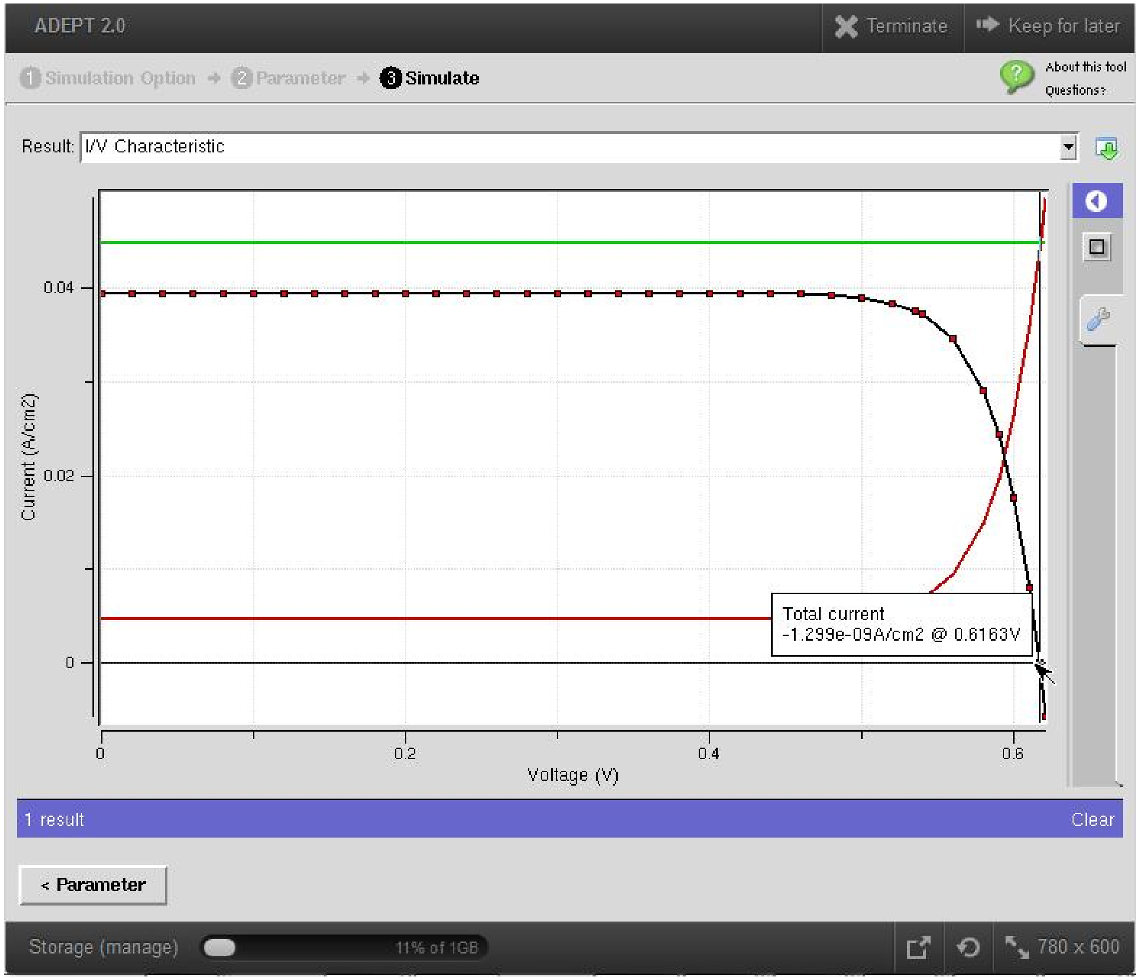
ADEPT: Output

- Carrier concentrations:



ADEPT: Output

- And finally, realistic I-V curves:



Next Class

- We will continue with electronic drift-diffusion modeling for other classes of electronics not amenable to analysis with ADEPT