

Special Topics on Basic EECS I Design Technology Co-Optimization

Lecture 16

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L16

Carrier densities at equilibrium

- Number of electrons

$$\int_{E_C}^{\infty} D(E) f(E) dE$$

- Density-of-states, $D(E) \propto \sqrt{E - E_C}$
- Distribution, $f(E)$. At equilibrium, $f(E)$ follows the Fermi-Dirac distribution:

$$f(E) = \frac{1}{1 + \exp \frac{E - E_F}{k_B T}} \approx \exp \left(-\frac{E - E_F}{k_B T} \right)$$

- Then, $\int_{E_C}^{\infty} D(E) f(E) dE \approx N_C \exp \left(-\frac{E_C - E_F}{k_B T} \right)$

Nonlinear Poisson equation

- The Gauss law within the electrostatic approximation

$$\nabla \cdot [-\epsilon(\mathbf{r})\nabla\phi] = \rho(\mathbf{r})$$

- The net charge density is given as

$$\rho(\mathbf{r}) = qp(\mathbf{r}) - qn(\mathbf{r}) + qN_{dop}^+(\mathbf{r})$$

- At equilibrium,

- We have $n(\mathbf{r}) = n(\phi(\mathbf{r}))$ and $p(\mathbf{r}) = p(\phi(\mathbf{r}))$.

- Then, the Gauss law reads:

$$\nabla \cdot [-\epsilon(\mathbf{r})\nabla\phi] = \rho(\mathbf{r}) = qp(\phi(\mathbf{r})) - qn(\phi(\mathbf{r})) + qN_{dop}^+(\mathbf{r})$$

- It is called the “nonlinear” Poisson equation.

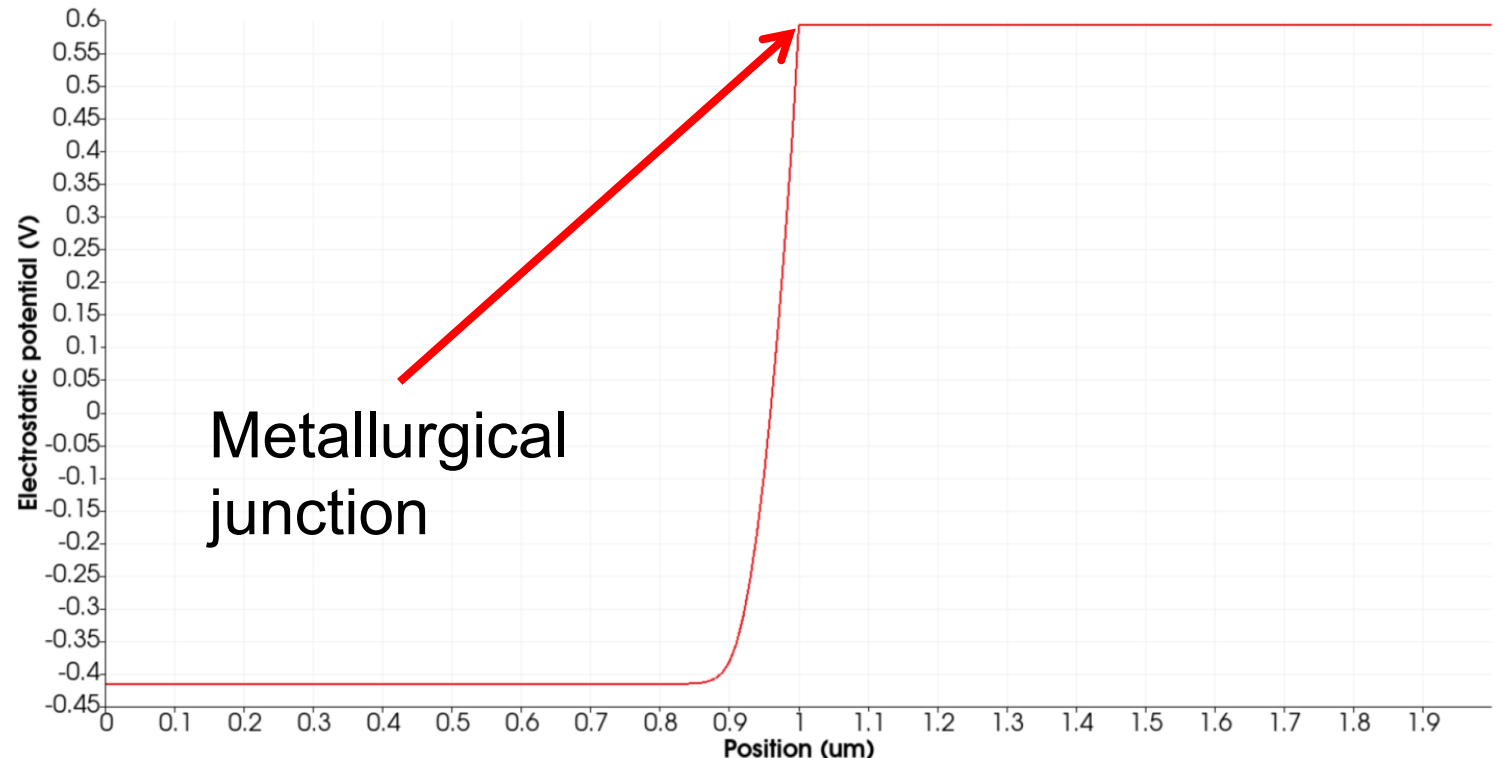
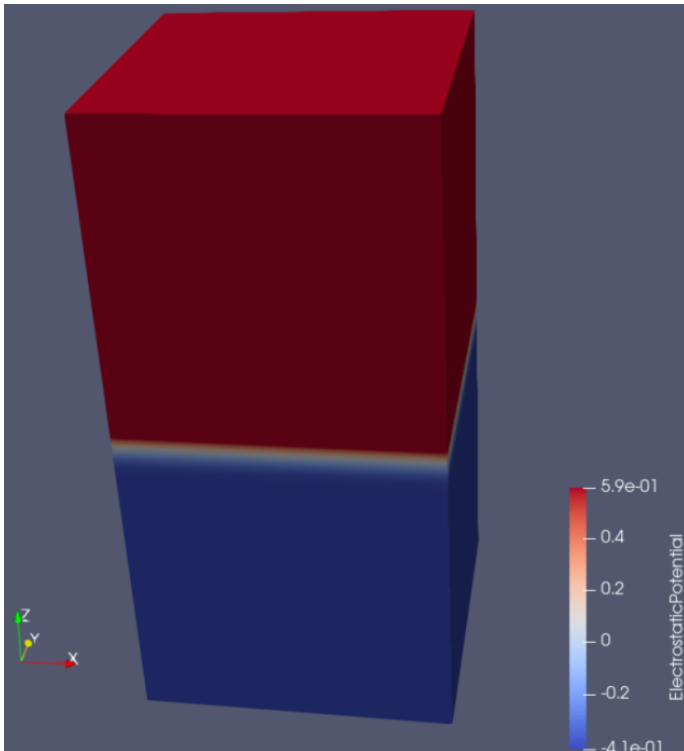
Equilibrium solution

- Load a structure and the nonlinear Poisson equation.
 - Our TA will send you the dbpath.

```
thing (type="device",name="pn") {  
  device (type="3d",areafactor=1.0) {  
    load (cgns="pn.cgns",dbpath="Here goes your dbpath."  
  }  
}  
  
property (thing="pn",model="effectiveintrinsicdensity",nobandgapnarrowing)  
  
law (name="eqlaw") {  
  equation (type="poisson",thing="pn")  
}  
  
solve (law="eqlaw",initialstep=1.0,plot,plotprefix="pn_equilibrium",cgns)
```

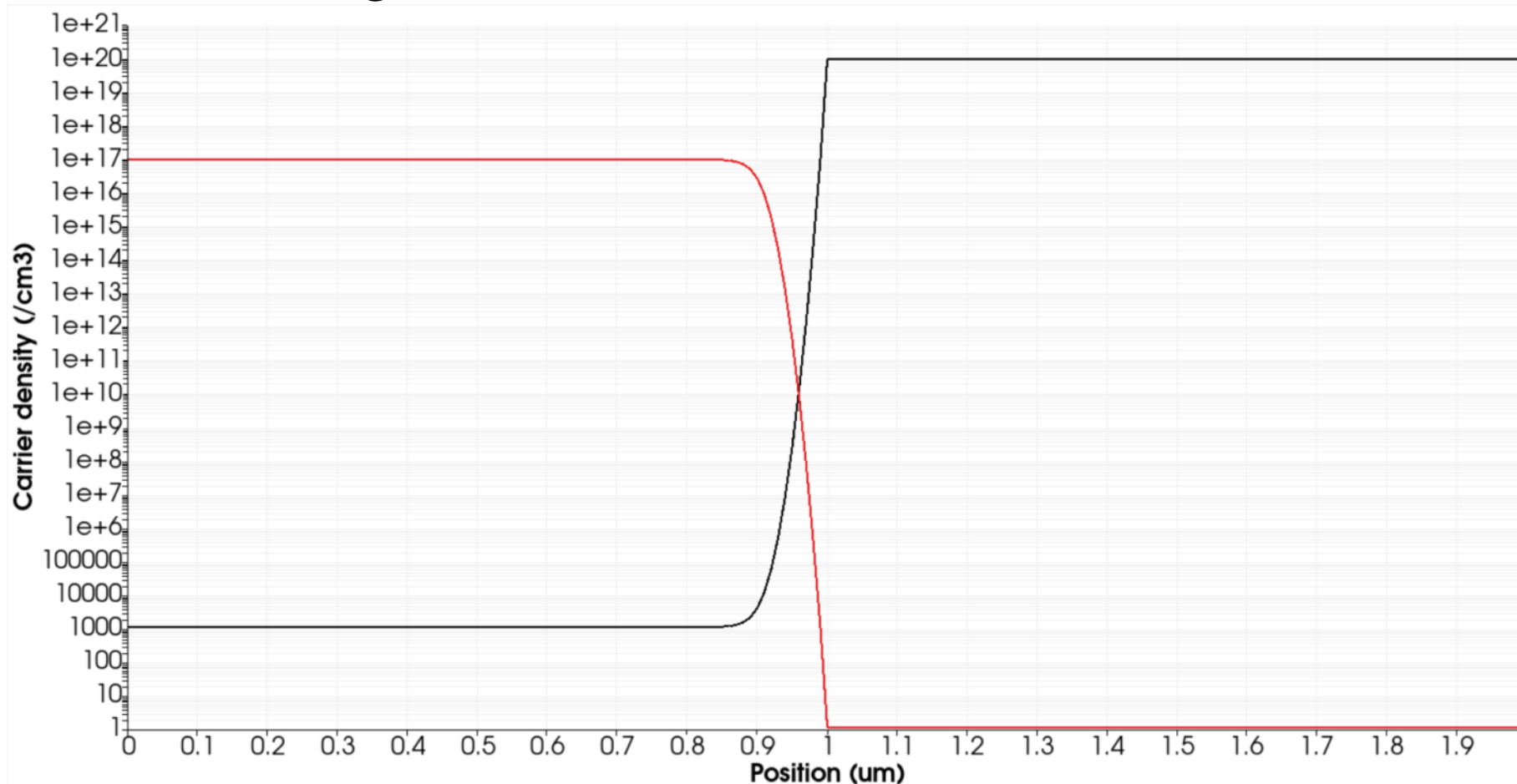
Electrostatic potential at equilibrium

- Visualization using Paraview
 - Values on the surface
 - Cutline (Again, watch “[Eng][TCAD2022] How to draw a cutline graph” for this purpose.)



Carrier densities

- Add more variables, eDensity and hDensity.
 - Draw a semi-logarithmic curve.



Construct a circuit to apply a voltage.

- A voltage source is needed.

- Create a PN junction. (We did it.)
- Create a voltage source (another `thing` statement)
- Connect them. (another `thing` statement)

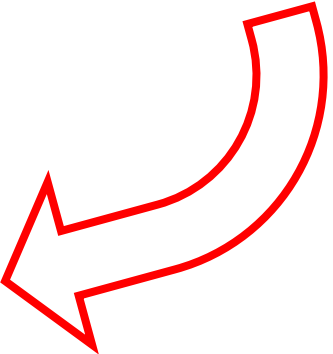
```
thing (type="lumped",name="battery") {  
    lumped (type="v",value=0.0)  
}
```

```
thing (type="circuit",name="circuit") {  
    circuit {  
        node (thing="gnd",name="GND")  
        node (thing="pn",contact="cathode",name="GND")  
        node (thing="pn",contact="anode",name="IN")  
        node (thing="battery",contact="0",name="GND")  
        node (thing="battery",contact="1",name="IN")  
    }  
}
```


Set the drift-diffusion model.

- Poisson equation, continuity equations, expressions for terminal currents, and Kirchhoff's current law
 - Therefore, we need additional equations.

```
law (name="eqlaw") {  
    equation (type="poisson", thing="pn")  
}  
  
law (name="dclaw") {  
    equation (type="poisson",    thing="pn")  
    equation (type="econtinuity", thing="pn")  
    equation (type="hcontinuity", thing="pn")  
    equation (type="contact",    thing="pn")  
    equation (type="virlc",      thing="battery")  
    equation (type="kirchhoff",  thing="circuit")  
}
```



Monitoring the IV curve

- We must specify the IV curve.
 - If not specified, there is no IV curve.
 - Only selected terminal quantities set by `book` statement are printed.

```
book (name="dc_iv", csv="dc_iv.csv") {  
    event (thing="pn", contact="cathode")  
    event (thing="pn", contact="anode")  
}
```

- The resultant csv file can be also visualized with Paraview. Watch “[Eng][TCAD2022] How to draw an IV curve” for visualization.

Bias ramping

- Increasing the voltage
 - It is done by changing a quantity (“voltage”) of the voltage source.
 - We cannot(?) abruptly change it from 0 to its final value.
 - Bias ramping is controlled by `initialstep`, `minstep`, and `maxstep`.

```
solve (law="dclaw",initialstep=0.001,maxstep=0.01,minstep=1e-6,plot,plotprefix="dc",cgns,book="dc_iv") {  
  goal (thing="battery",quantity="voltage",value=0.7)  
}
```

- When the simulation is finished, the output file “dc.cgns” represents a device biased at 0.7 V.

Entire input file (1)

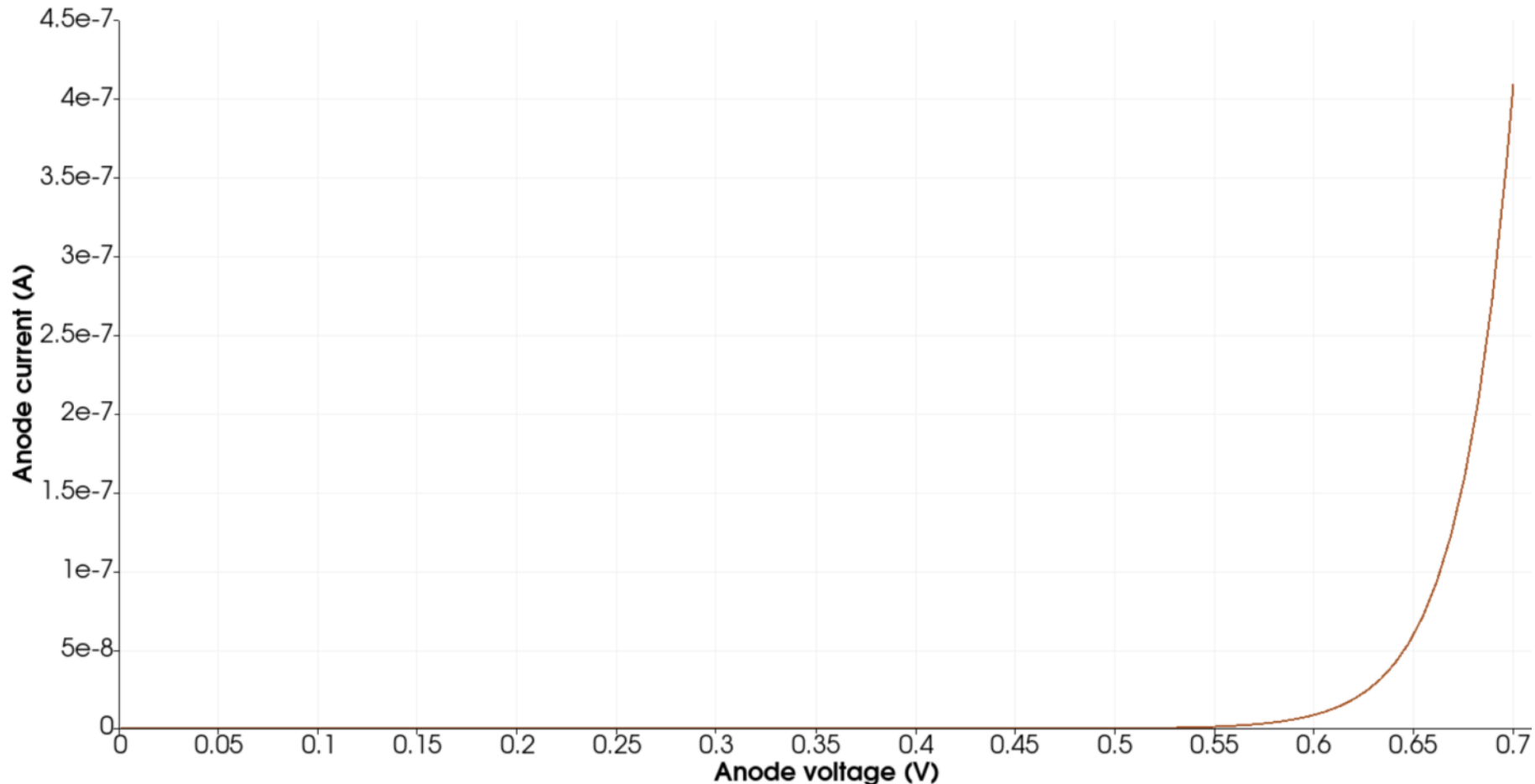
```
thing (type="device",name="pn") {  
    device (type="3d",areafactor=1.0) {  
        load (cgns="pn.cgns",dbpath="Here goes your dbpath.")  
    }  
}  
  
thing (type="lumped",name="battery") {  
    lumped (type="v",value=0.0)  
}  
  
thing (type="circuit",name="circuit") {  
    circuit {  
        node (thing="gnd",name="GND")  
        node (thing="pn",contact="cathode",name="GND")  
        node (thing="pn",contact="anode",name="IN")  
        node (thing="battery",contact="0",name="GND")  
        node (thing="battery",contact="1",name="IN")  
    }  
}  
  
property (thing="pn",model="effectiveintrinsicdensity",nobandgapnarrowing)
```

Entire input file (2)

```
law (name="eqlaw") {  
    equation (type="poisson",thing="pn")  
}  
  
law (name="dclaw") {  
    equation (type="poisson",    thing="pn")  
    equation (type="econtinuity",thing="pn")  
    equation (type="hcontinuity",thing="pn")  
    equation (type="contact",    thing="pn")  
    equation (type="virlc",      thing="battery")  
    equation (type="kirchhoff",  thing="circuit")  
}  
  
book (name="dc_iv",csv="dc_iv.csv") {  
    event (thing="pn",contact="cathode")  
    event (thing="pn",contact="anode")  
}  
  
solve (law="eqlaw",initialstep=1.0,plot,plotprefix="pn_equilibrium",cgns)  
  
solve (law="dclaw",initialstep=0.001,maxstep=0.01,minstep=1e-6,plot,plotprefix="dc",cgns,book="dc_iv") {  
    goal (thing="battery",quantity="voltage",value=0.7)  
}
```

IV curve, forward

- From 0 V to 0.7 V
 - Rectifying behavior, as expected



Homework#16

- Due: 08:00 on Nov. 12
- Submit a report through the GIST LMS system.
 - Simulate the IV characteristics of our PN junction. (Forward and reverse IV curves)

Thank you!