Practical Physics-Based Device Modeling: The Numerical Boltzmann/Spherical Harmonic Method

Neil Goldsman
Electrical and Computer Engineering
University of Maryland
College Park, MD USA

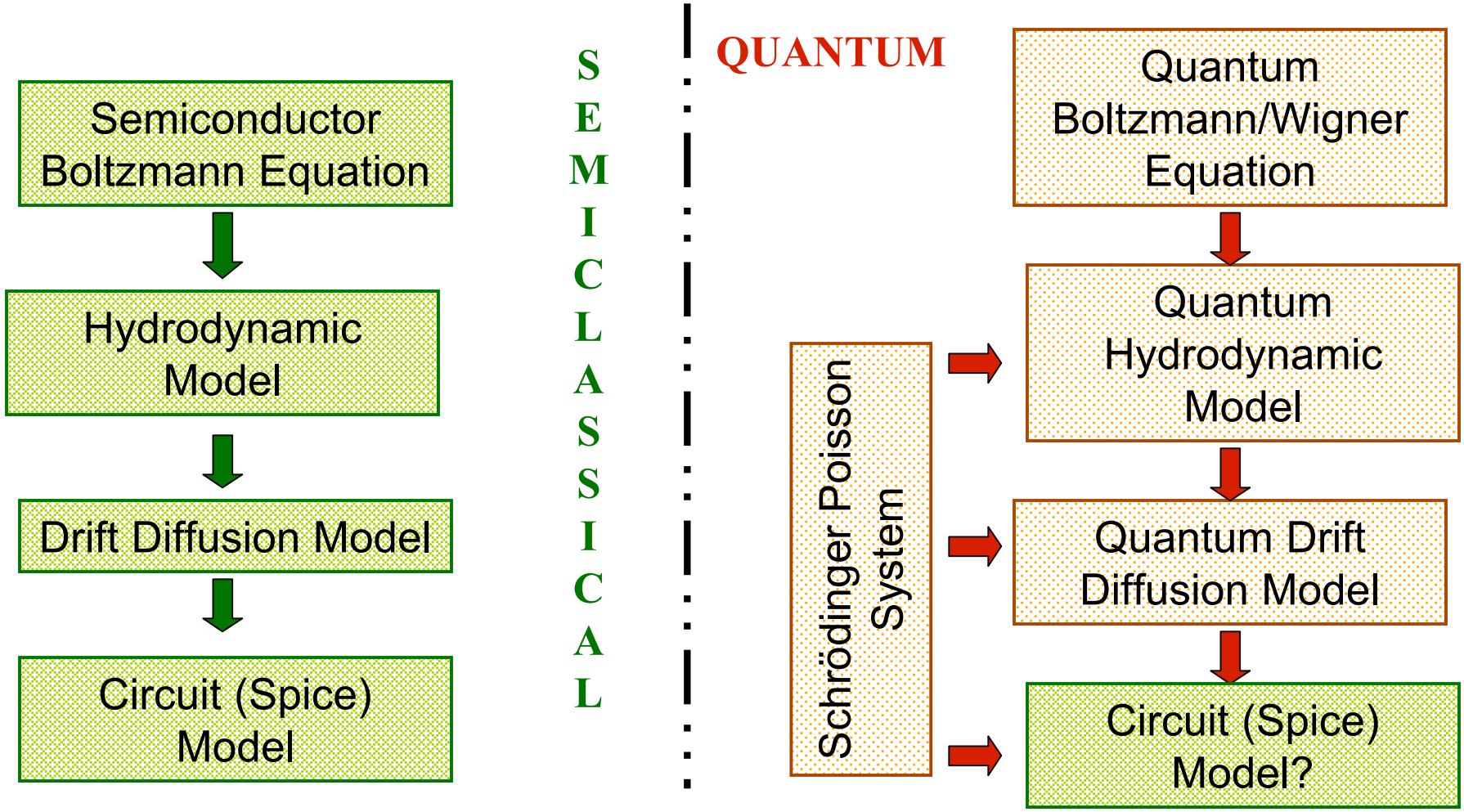
Outline

- Overview of Device Simulation
  - Benefits
  - Approaches
- Numerical Boltzmann/Spherical Harmonic Method: A Balanced Approach
  - Formulation and Application of Semiclassical to MOSFETs
  - Quantum Correction (Wigner)
  - Transient Application to BJT

Benefits of Device Simulation

- Allows you to probe inside device where measurements can not be made.
- Explore new experimental devices and device phenomena without fabricating device.
- Educate researchers, engineers and students to expand the frontiers of mathematical and computational skills germane to microelectronics.
- Help develop CAD tools so industry can continue its march forward in the miniaturization of electronic devices and circuits.

Semiconductor Simulation Models: Hierarchy



Semiclassical Models

All contain Poisson Equation + Transport Equation

Boltzmann Transport Equation Model:

$$\nabla^2\phi = \frac{q}{\varepsilon_s}\left[\int f(\vec{r},\vec{k},t)d\vec{k} - p(\vec{r},t) + N_A(\vec{r}) - N_D(\vec{r})\right]$$

$$\frac{\partial f}{\partial t} + \frac{1}{\hbar}\nabla_{\vec{k}}\varepsilon(\vec{k})\cdot\nabla_{\vec{r}} f + \frac{q}{\hbar}\nabla_{\vec{r}} V(\vec{r},t)\cdot\nabla_{\vec{k}} f = \left(\frac{\partial f}{\partial t}\right)_{coll}$$

$$\vec{r}\in\mathbf{R}^3, \vec{k} = (k_x, k_y, k_z)$$

Hydrodynamic Model:

$$\nabla^2\phi = -\frac{q}{\varepsilon}\left(-n + p + N_D^+ - N_A^-\right)$$

$$q\frac{\partial n}{\partial t} = \nabla\cdot\vec{J}_n - q(R-G)$$

$$\frac{\partial\vec{v}}{\partial t} + (\nabla\cdot\vec{v})\vec{v} + \frac{k_B}{m^* n}\nabla(nT) - \frac{q}{m^*}\nabla V = C_{\vec{u}}$$

Drift-Diffusion Model:

$$\nabla^2\phi = -\frac{q}{\varepsilon}\left(-n + p + N_D^+ - N_A^-\right)$$

$$q\frac{\partial n}{\partial t} = \nabla\cdot\vec{J}_n - q(R-G)$$

$$\vec{J}_n = -qn\mu_n\nabla\phi + qD_n\nabla n$$

Transport equations are shown here only for electrons. Transport equations for holes are analogous and understood.

The Model Trade-Offs

CAD tools usually represent a trade-off between physical rigor and computational efficiency.

Generally speaking, the more physically rigorous, the less computationally efficient.

Drift-Diffusion: Most CPU Efficient (Commercial Codes)

Monte Carlo: Least CPU Efficient

One of my personal goals in device simulation is to optimize this trade-off.

Numerical Boltzmann/Spherical Harmonics Method

Boltzmann-Device Model

Advantages:

- Gives distribution function for entire device
- From distribution function virtually all device characteristics can be obtained.
- Explicitly includes scattering
- Expandable to quantum domain (Schrodinger or Wigner).

Difficulties:

- Boltzmann equation is 7 dimensional (3 real-space, 3 momentum, 1 time)
- Direct discretization virtually impossible due to high dimensionality.
- Collision integral can cause global coupling of discretized system.

Boltzmann-Device Model

Poisson Equation:

$$\nabla_{\vec{r}}^2 V(\vec{r}) = \frac{q}{\varepsilon_s}\left[\int f(\vec{r},\vec{k},t)\,d\vec{k} - p(\vec{r},t) + N_A(\vec{r}) - N_D(\vec{r})\right]$$

Boltzmann Transport Equation:

$$\frac{\partial f}{\partial t} + \frac{1}{\hbar}\nabla_{\vec{k}}\varepsilon \cdot \nabla_{\vec{r}} f - \frac{q}{\hbar}\nabla_{\vec{r}} V(\vec{r}) \cdot \nabla_{\vec{k}} f = \left(\frac{\partial f}{\partial t}\right)_{coll}$$

Hole-Current Continuity Equation:

$$\frac{\partial p(\vec{r},t)}{\partial t} + \nabla_{\vec{r}} \cdot \left[\mu_p p(\vec{r}) \nabla_{\vec{r}} \phi(\vec{r}) + \mu_p V_t \nabla_{\vec{r}} p(\vec{r})\right] = R(\phi, n, p) - G_{ii}(n, p)$$

Solve the system for :

- Potential : $\phi(\vec{r},t)$
- Electron Distribution Function : $f(\vec{r},\vec{k},t)$
- Hole Concentration : $p(\vec{r},t)$

Collision Term

$$\left[\frac{\partial f(\vec{r},\vec{k})}{\partial t}\right]_{coll} = \frac{V}{(2\pi)^3}\sum_{l,m,i}\int\left[f(\vec{r},\vec{k}',t)S_i(\vec{k}',\vec{k}) - f(\vec{r},\vec{k},t)S_i(\vec{k},\vec{k}')\right]d^3\vec{k}'$$

The summation over *i* represents the different scattering processes which occur in MOSFETs.

$s_i(\vec{k},\vec{k}')$ = the transition probability per unit time for the ith type of scattering.

The different scattering mechanisms incorporated in the collision term can be :

- **Optical Phonon Scattering**
- **Acoustic Phonon Scattering**
- **Surface Roughness Scattering**
- **Ionized Impurity Scattering**
- **SHR Recombination**
- **Impact Ionization**

BTE: Spherical Harmonics Method

- Solution to 'Curse of Dimensionality Problem'
- Represent Distribution Function ***f(r,k,t)*** using Spherical Harmonic basis functions.
- Reduces dimension from 7 to 5 for 3D transient

$$f\left(\vec{r},\vec{k},t\right)=\sum_{l,m} f_l^m\left(\vec{r},k,t\right)Y_l^m\left(\theta,\phi\right)$$

$\vec{r}$ $\Rightarrow$ Position Vector

$\vec{k}$ $\Rightarrow$ Wave Vector

$Y_l^m(\theta,\phi)$ $\Rightarrow$ Spherical Harmonics

$f_l^m(\vec{r},k,t)$ $\Rightarrow$ Unknown Expansion Coefficients

$k=|\vec{k}|$ $\Rightarrow$ Magnitude of the wave vector $\vec{k}$

θ,ϕ $\Rightarrow$ Polar and Azimuthal angles of wave vector $\vec{k}$

$l=0,1,2,\ldots.$

$m=-l$ to $+l$

System of Equations for f_l^m

Boltzmann Transport Equation:

$$\frac{\partial f}{\partial t}+\frac{1}{\hbar}\nabla_{\vec{k}}\varepsilon\cdot\nabla_{\vec{r}}f-\frac{q}{\hbar}\nabla_{\vec{r}}V(\vec{r})\cdot\nabla_{\vec{k}}f=\left(\frac{\partial f}{\partial t}\right)_{coll}$$

Spherical Harmonic Form for BTE:

$$\frac{\partial f_l^m}{\partial t}+\sum_{i=1}^{3}\left\{\begin{aligned}&v(\varepsilon)\left[\frac{\partial}{\partial x_i}-qE_i(\vec{r})\left(\frac{\partial}{\partial\varepsilon}-\frac{(l-1)}{2}\frac{\gamma'(\varepsilon)}{\gamma(\varepsilon)}\right)\right]\hat{a}_i^-\\&\qquad+v(\varepsilon)\left[\frac{\partial}{\partial x_i}-qE_i(\vec{r})\left(\frac{\partial}{\partial\varepsilon}+\frac{(l+2)}{2}\frac{\gamma'(\varepsilon)}{\gamma(\varepsilon)}\right)\right]\hat{a}_i^+\end{aligned}\right\}f_l^m=\left[\frac{\partial f_l^m}{\partial t}\right]_{coll}$$

$\vec{E}=(E_1,E_2,E_3)\Rightarrow$ Electric Field

$\varepsilon \Rightarrow$ Energy

$\vec{x}=(x_1,x_2,x_3) \Rightarrow$ Position Vector

$v(\varepsilon)=|\vec{v}(\varepsilon)| \Rightarrow$ Group Velocity

$\gamma(\varepsilon)=p^2/2m^* \Rightarrow$ General Dispersion Relation

$\hat{a}_i^+,\hat{a}_i^- \Rightarrow$ Operators operating on f_l^m

Differential Difference Equation Form

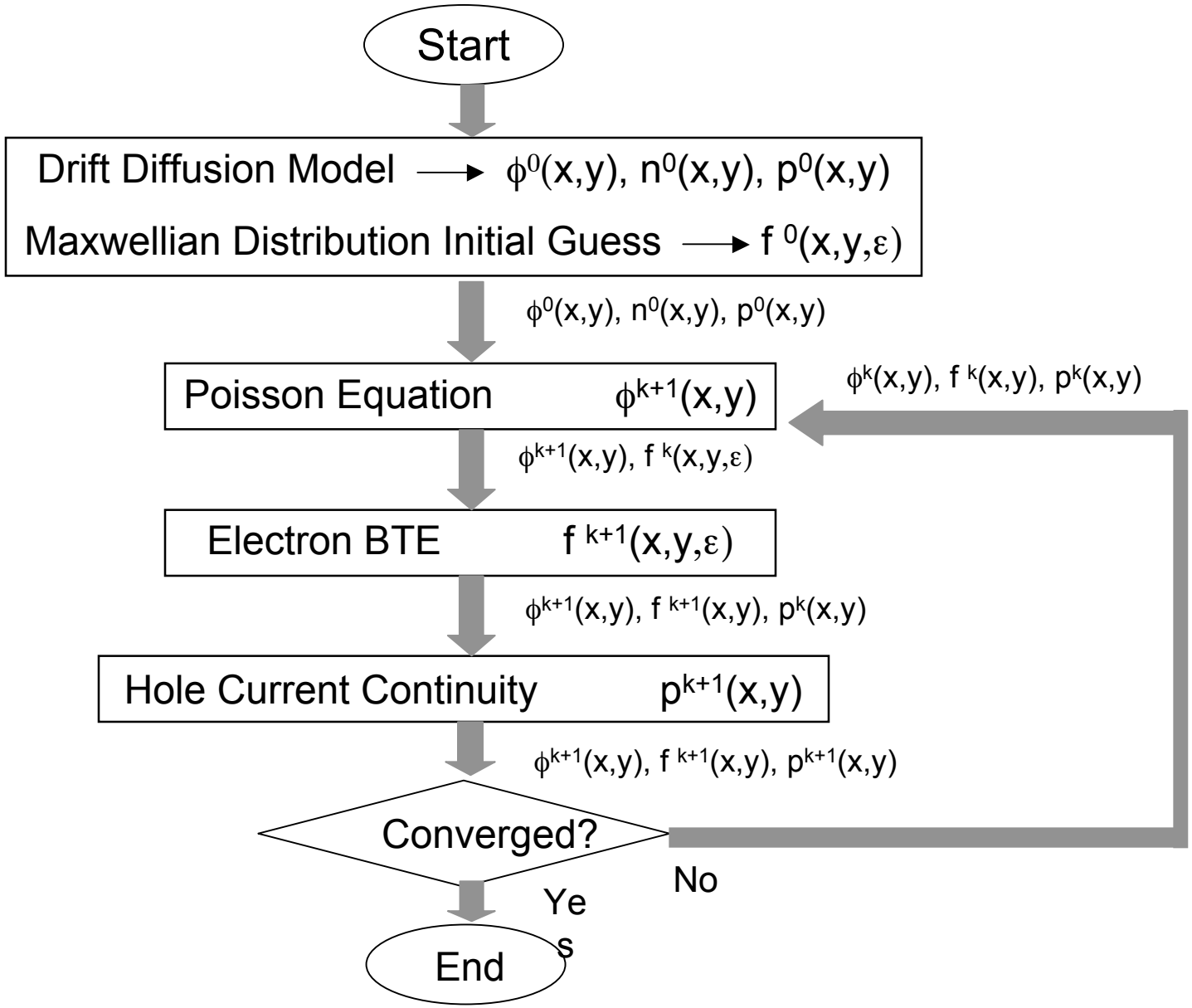
- The equations for each unknown coefficient $f_l^m(r,\varepsilon)$ described in the SH form of BTE are truncated.
- Substitute equations for f_1^{-1}, f_1^0, f_1^1 into equation for f_0^0
- We get a 3-D self-adjoint, differential difference equation from the BTE:
- Solve SH formulated BTE numerically: finite diffs, CG

$$\frac{\partial f_0^0}{\partial t} + \sum_{i=1}^{3} \frac{\partial}{\partial x_i}\left(\frac{\gamma^{3/2}\tau}{\gamma'}\frac{\partial f_0^0}{\partial x_i}\right) + \frac{3m^*}{2}\gamma^{1/2}\gamma'\left(\frac{\partial f_0^0}{\partial t}\right)_{coll} = 0$$

Where, the collision term is a summation over all the scattering mechanisms:

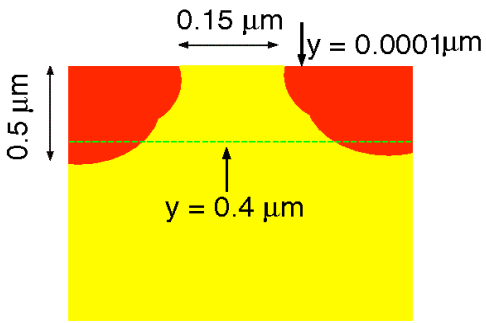
$$\left(\frac{\partial f_0^0}{\partial t}\right)_{coll} = \left(\frac{\partial f_0^0}{\partial t}\right)_{opt} + \left(\frac{\partial f_0^0}{\partial t}\right)_{ac} + \left(\frac{\partial f_0^0}{\partial t}\right)_{sr} + \left(\frac{\partial f_0^0}{\partial t}\right)_{ion} + \left(\frac{\partial f_0^0}{\partial t}\right)_{ii} + \left(\frac{\partial f_0^0}{\partial t}\right)_{SHR}$$

Flowchart

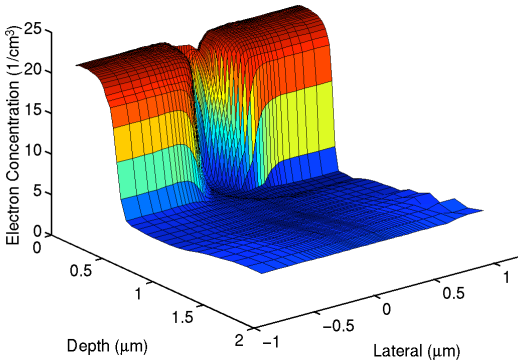

Start
Drift Diffusion Model → $\phi^0(x,y)$, $n^0(x,y)$, $p^0(x,y)$
Maxwellian Distribution Initial Guess → $f^0(x,y,\varepsilon)$
$\phi^0(x,y)$, $n^0(x,y)$, $p^0(x,y)$
Poisson Equation $\phi^{k+1}(x,y)$
$\phi^k(x,y)$, $f^k(x,y)$, $p^k(x,y)$
$\phi^{k+1}(x,y)$, $f^k(x,y,\varepsilon)$
Electron BTE $f^{k+1}(x,y,\varepsilon)$
$\phi^{k+1}(x,y)$, $f^{k+1}(x,y)$, $p^k(x,y)$
Hole Current Continuity $p^{k+1}(x,y)$
$\phi^{k+1}(x,y)$, $f^{k+1}(x,y)$, $p^{k+1}(x,y)$
Converged?
No
Yes
End

Numerical Boltzmann/Spherical Harmonic Device CAD Results: Device Structure and Distribution Function

MOS Cross Section

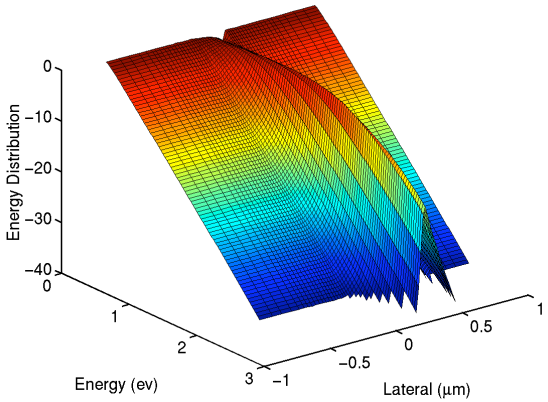


Electron Concentration

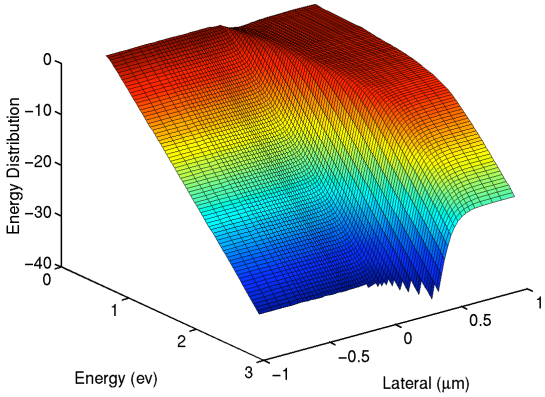


Distribution Function

Y=0.0001µm

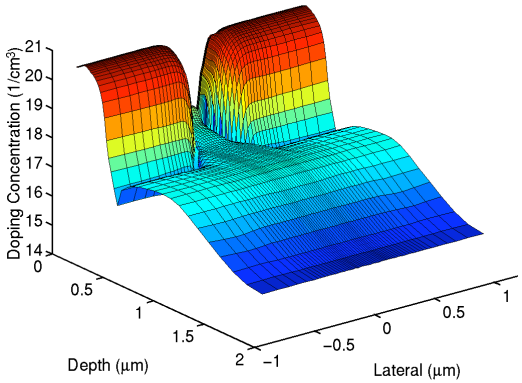


Y=0.4µm

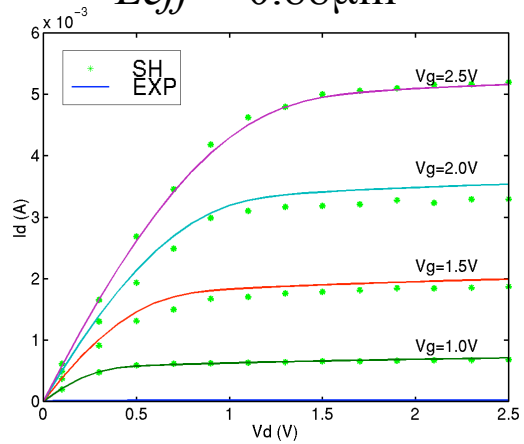


Numerical Boltzmann/Spherical Harmonic Device CAD Results: Benchmark I-V with Experiment

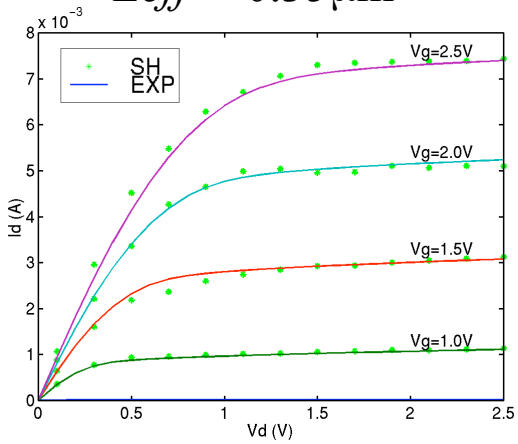
Doping Profile



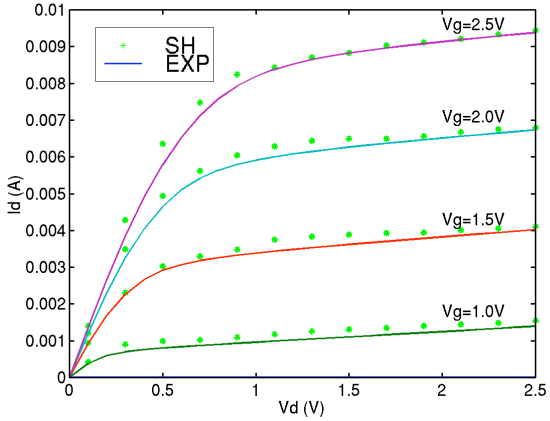
Leff = 0.88μm



Leff = 0.35μm



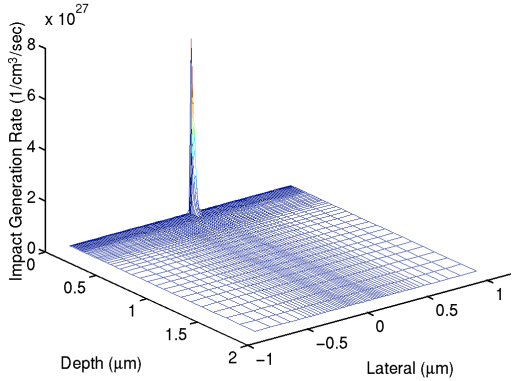
Leff = 0.15μm



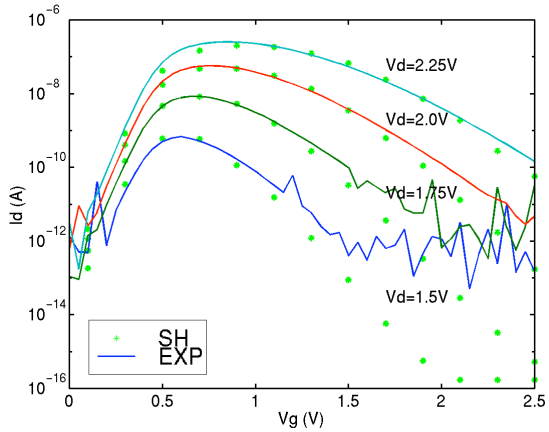
Numerical Boltzmann/Spherical Harmonic Device CAD Results: Impact Ionization and Substrate Current

Agreement with experiment: No fitting parameters!

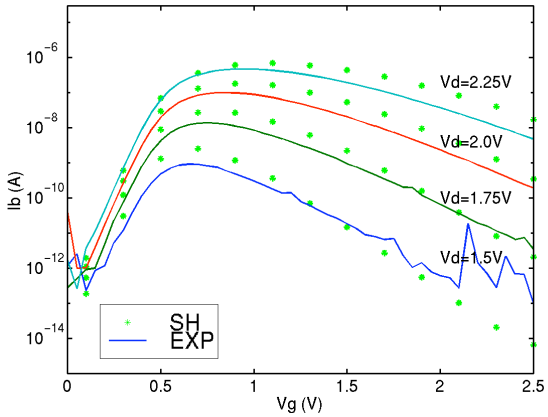
Generation Rate



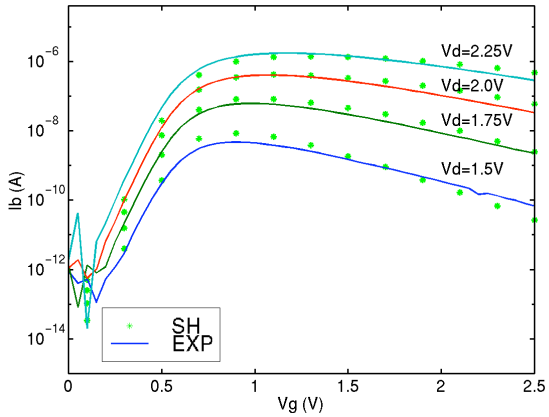
Leff = 0.88μm



Leff = 0.35μm



Leff = 0.15μm



Gate Current: Mathematical Model

The final gate leakage current will be the summation of the tunneling and thermionic current

$$J_{gate}(x) = J_{tu}(x) + J_{th}(x)$$

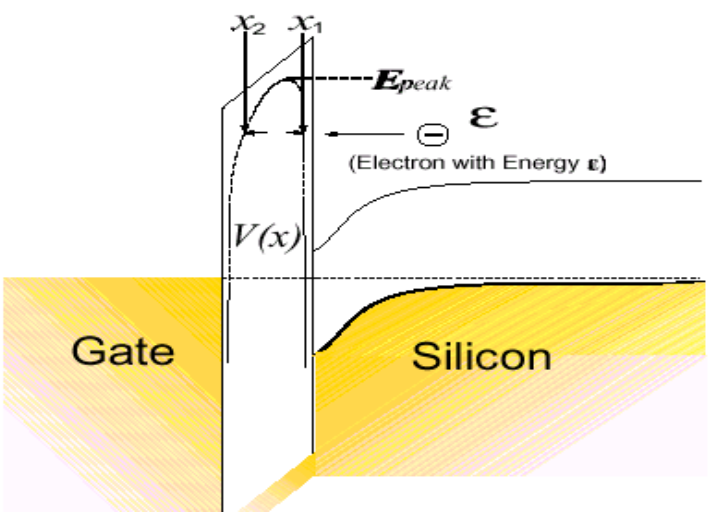
Where

Tunneling current

$$J_{tu}(x) = \int_0^{E_{peak}} f(\xi, x) g(\xi) v_{\perp}(\xi) T_{tun}(\xi, x) d\xi$$

Thermionic current

$$J_{ther}(x) = \int_{E_{peak}}^{\infty} f(\xi, x) g(\xi) v_{\perp}(\xi) T_{ther}(\xi, x) d\xi$$



J_{gate} = Gate Current Density

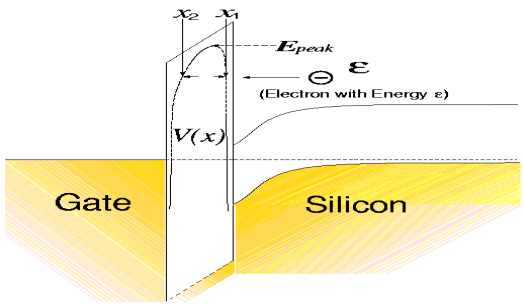
f = Distribution Function

g = Density of States

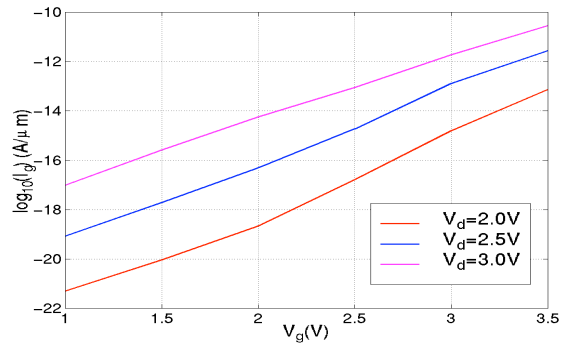
T_{tun} = Tunneling Probability

T_{ther} = Thermionic Probability

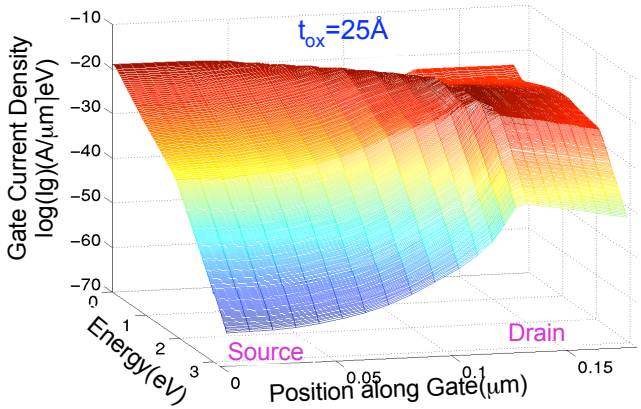
Numerical Boltzmann/Spherical Harmonic Device CAD Results: Gate Tunneling and Thermal Emission Current



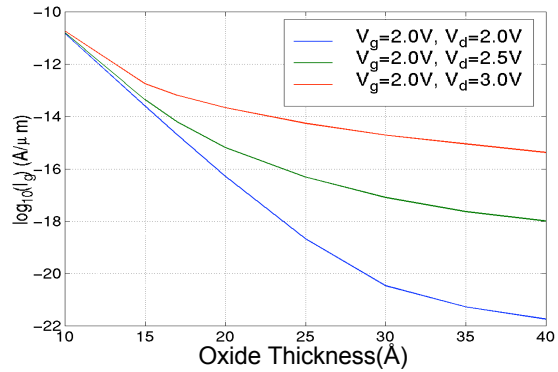
I_g vs V_g, V_d



I_g vs V_g, V_d

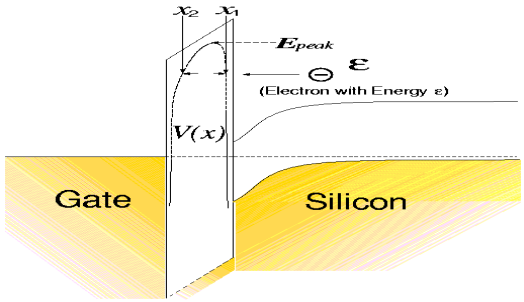


I_g vs Position and Energy



I_g vs Oxide Thickness

Extending the Numerical Boltzmann Spherical Harmonic to the Quantum Domain



I_g vs V_g, V_d

Spherical Harmonics

Boltzmann/Wigner Equation Method

Quantum Correction

Keeping only the first order expansion of potential, the Boltzmann/Wigner transport equation reduces to the Semiclassical Boltzmann Transport Equation.

The higher order terms are hence the Quantum Correction to the BTE. The potential expansion can be truncated at the first two terms as the higher order terms quickly become negligible for many electronic systems.

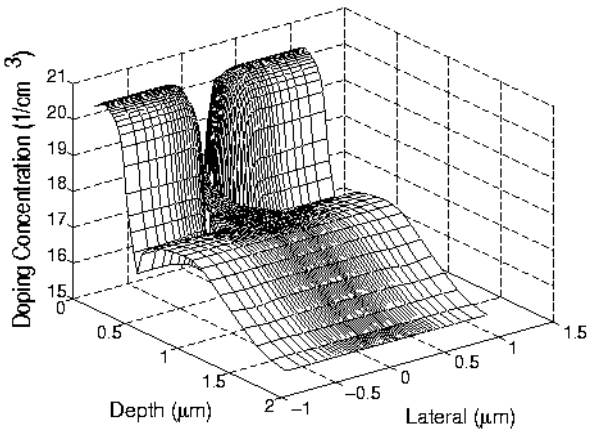
The STEADY STATE BOLTZMANN/WIGNER EQUATION CAN NOW BE WRITTEN AS:

Quantum Correction Term

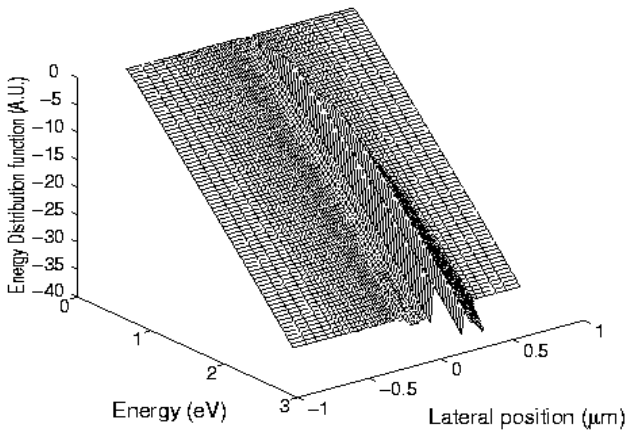
$$\frac{1}{\hbar}\nabla_{\vec{k}}\varepsilon\cdot\nabla_{\vec{r}}w-\frac{q}{\hbar}\nabla_{\vec{k}}V\cdot\nabla_{\vec{r}}w-\frac{q}{24\hbar}\left(\nabla_{\vec{k}}\cdot\nabla_{\vec{r}}\right)^{3}V\left(\vec{r}\right)w=\left(\frac{\partial w}{\partial t}\right)_{coll}$$

Quantum Effects: Boltzmann/Wigner Results

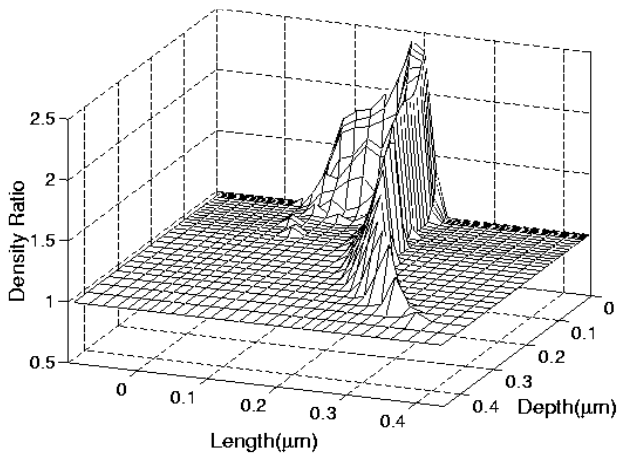
Doping profile



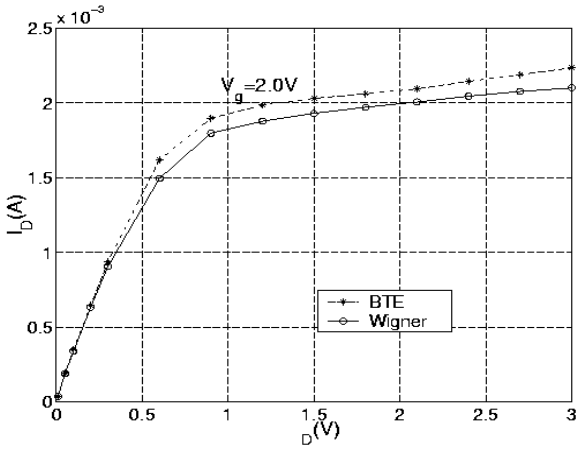
Quantum Dist. Fn.



Carrier Con. Ratio: Class/QM



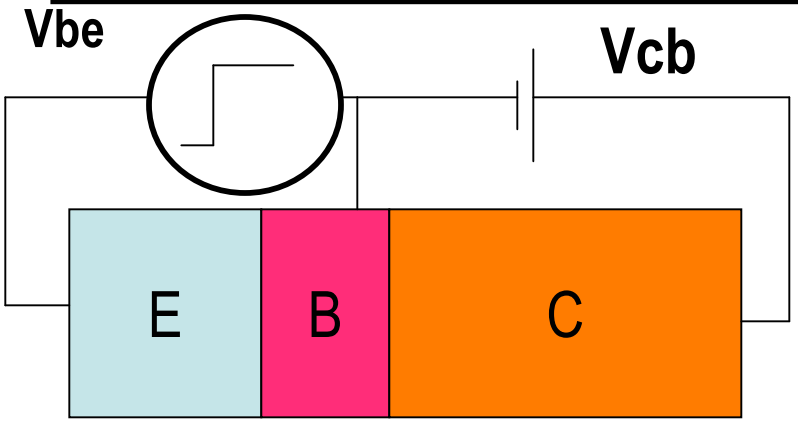
I~V Comparison



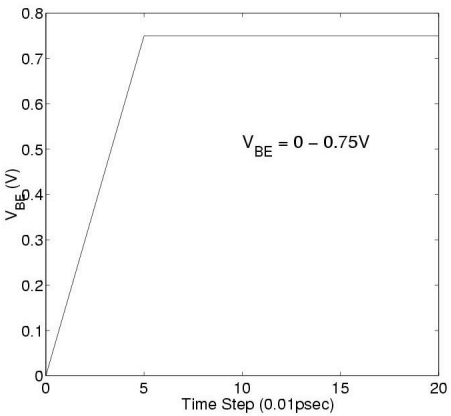
Extending the Numerical Boltzmann Spherical Harmonic to the Transient Regime

Transient Spherical Harmonics Boltzmann Equation Method

Transient Numerical Boltzmann/Spherical Harmonic BJT Simulation

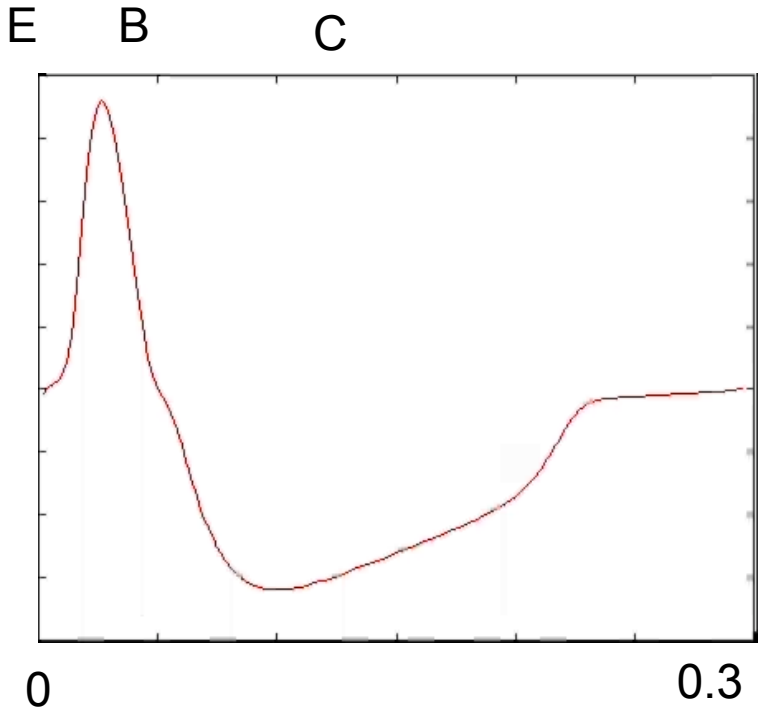


BJT Structure: 50nm Base



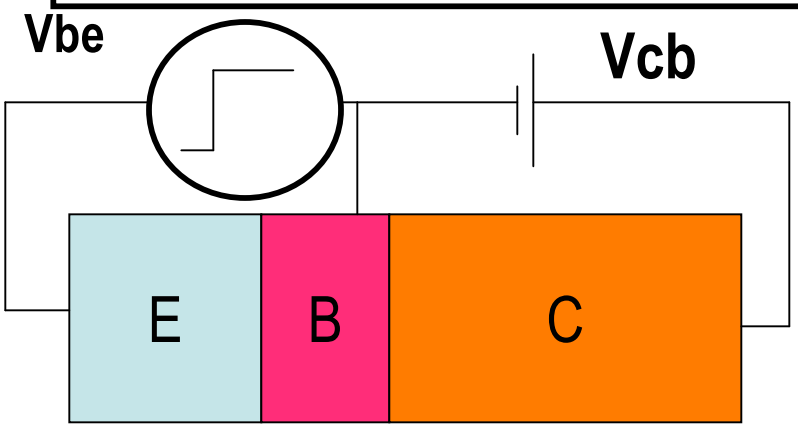
Input Signal: 20 psec step

E

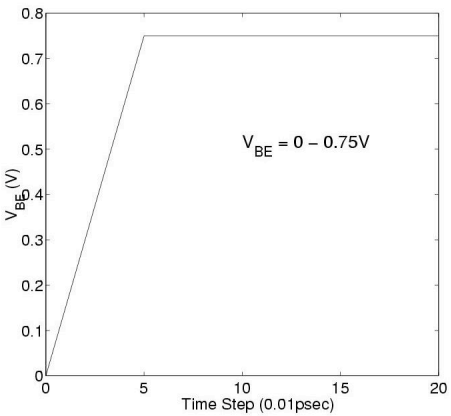


Electric Field vs Position (_m)

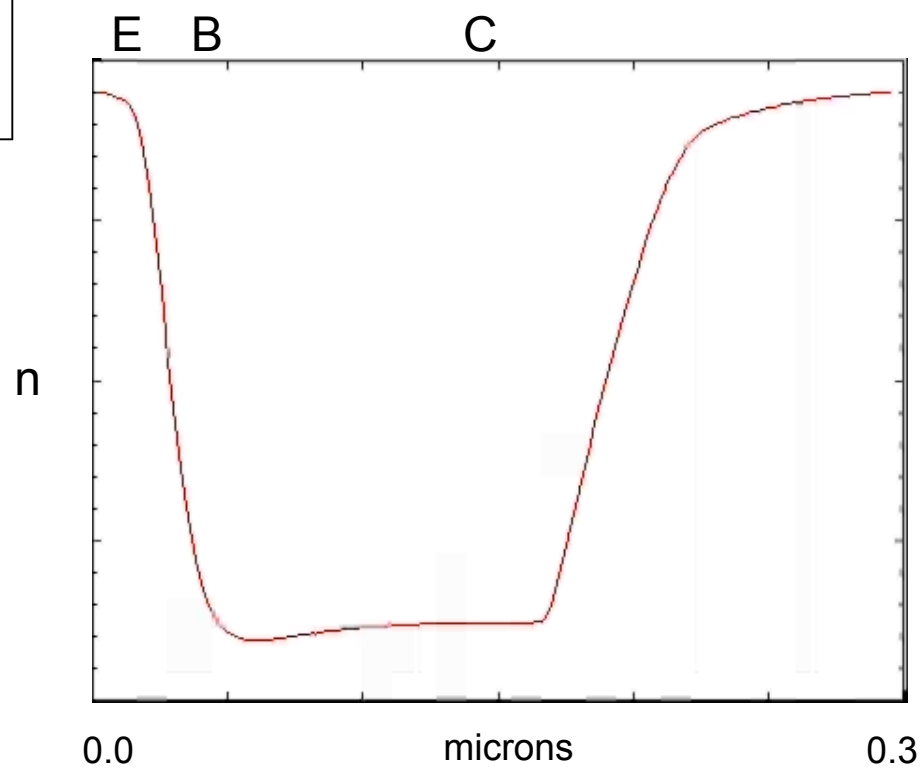
Transient Numerical Boltzmann/Spherical Harmonic BJT Simulation



BJT Structure: 50nm Base

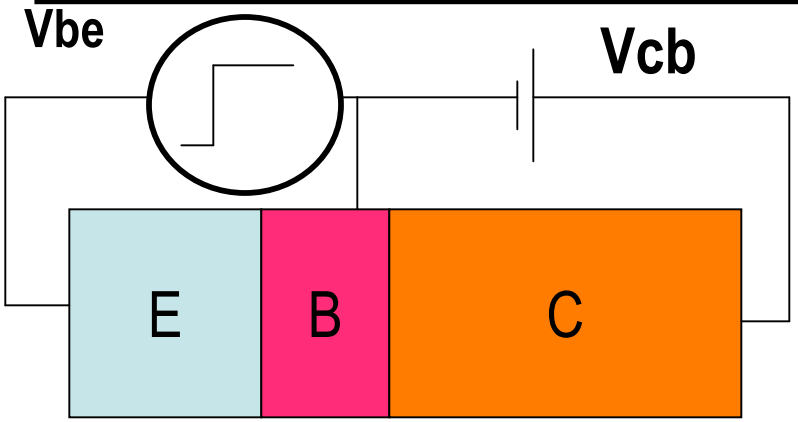


Input Signal: 20 psec step

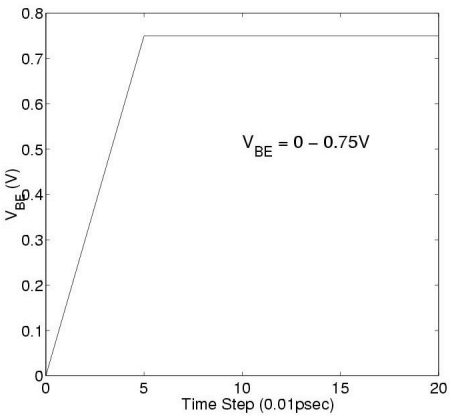


Electron Concentration (logscale) vs Position

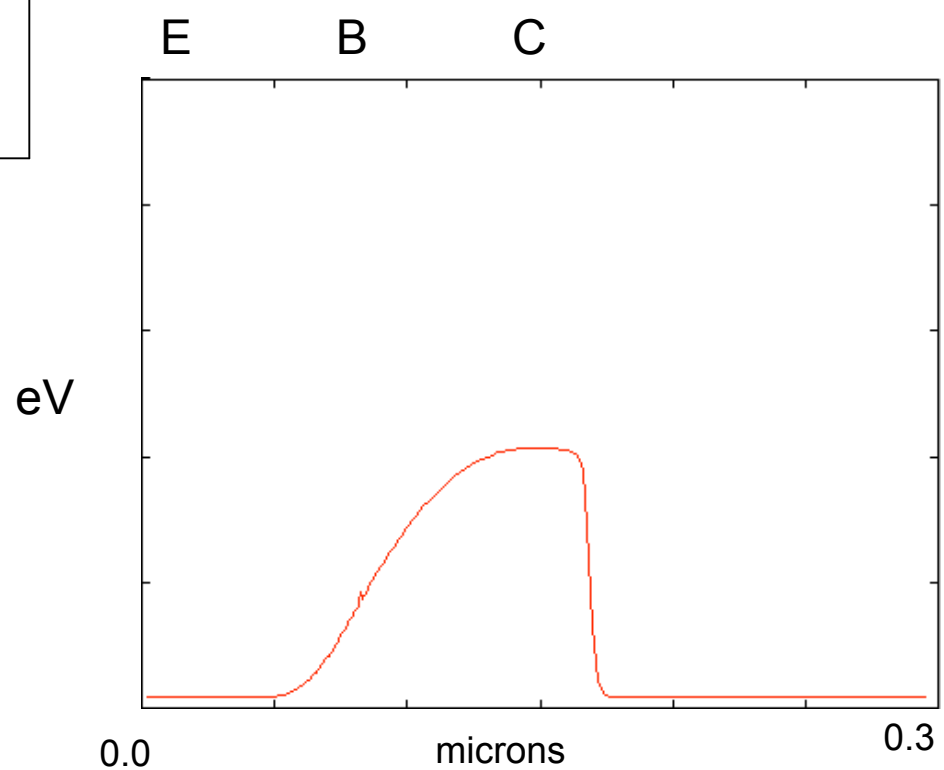
Transient Numerical Boltzmann/Spherical Harmonic BJT Simulation



BJT Structure: 50nm Base

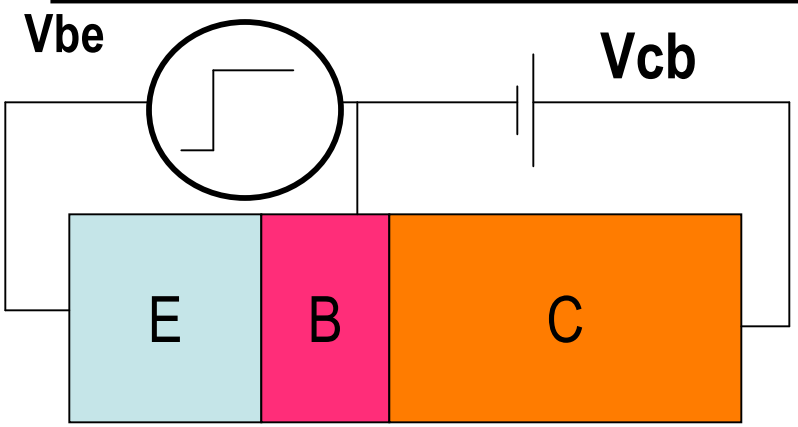


Input Signal: 20 psec step

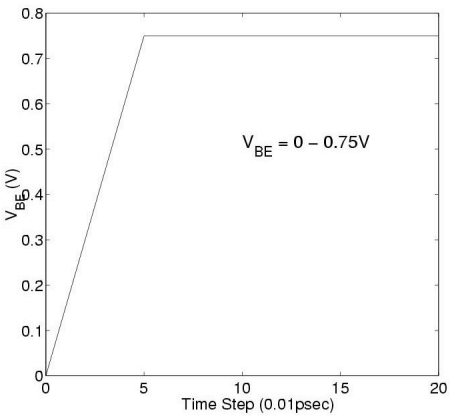


Average Electron Energy vs Position

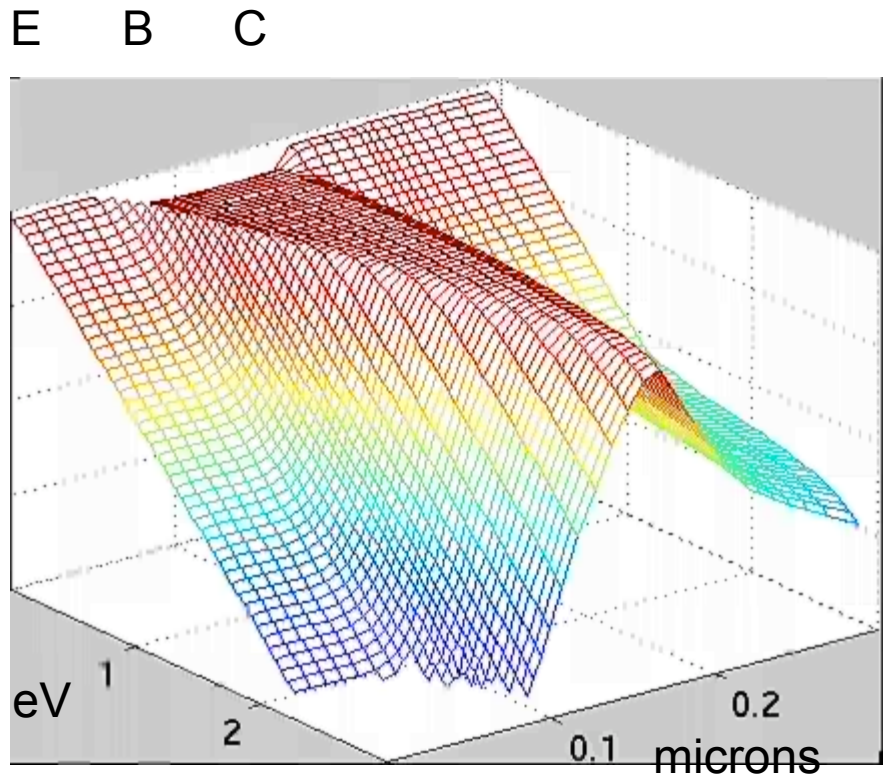
Transient Numerical Boltzmann/Spherical Harmonic BJT Simulation



BJT Structure: 50nm Base

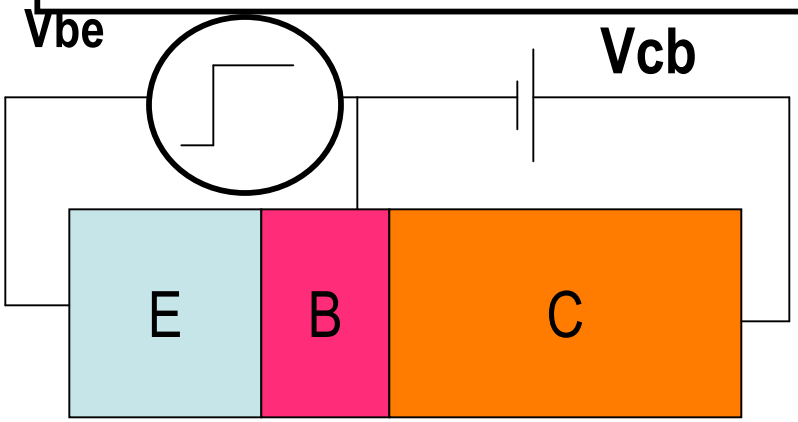


Input Signal: 20 psec step

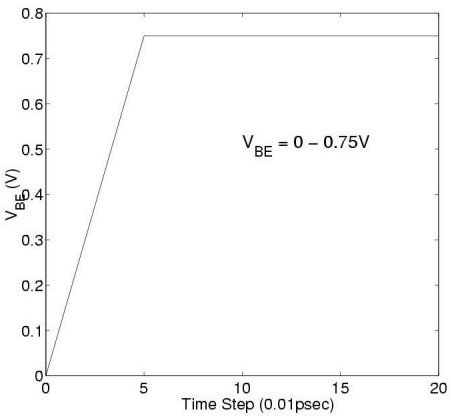


Distribution Function vs Position & Energy

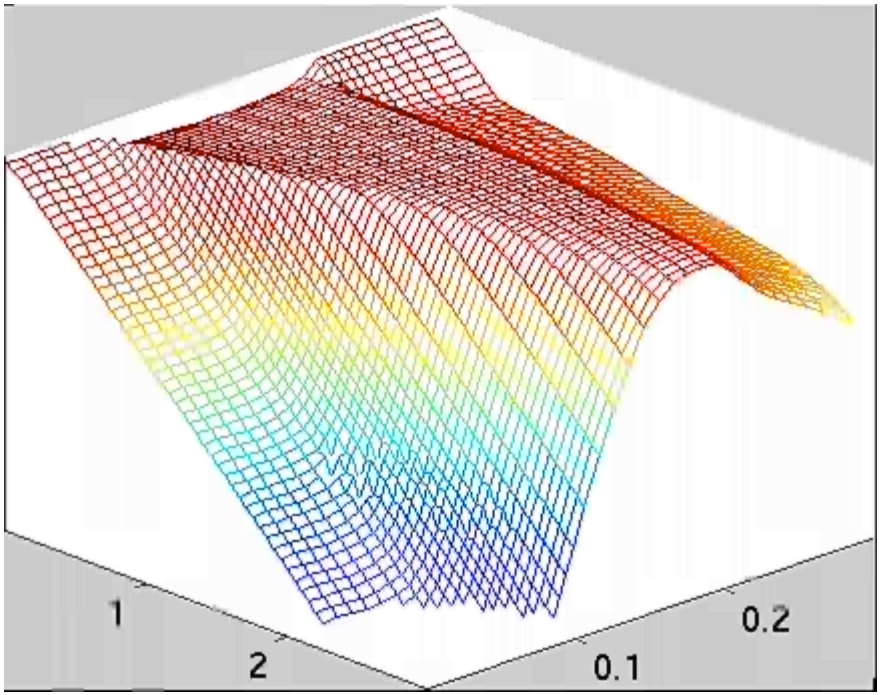
Transient Numerical Boltzmann/Spherical Harmonic BJT Simulation



BJT Structure: 50nm Base



Input Signal: 20 psec step



Summary

- In hierarchy of models, Numerical Boltzmann gives good tradeoff between accuracy and efficiency (1000 times faster than Monte Carlo)
- Numerical Boltzmann excellent for places where distribution function is required (impact ionization, gate leakage current, reliability).
- As devices shrink to nanoscale, quantum effects becoming very important, use either Wigner, density gradient or coupled Schrodinger
- Transient very important as well with clock speeds approaching 10GHz.