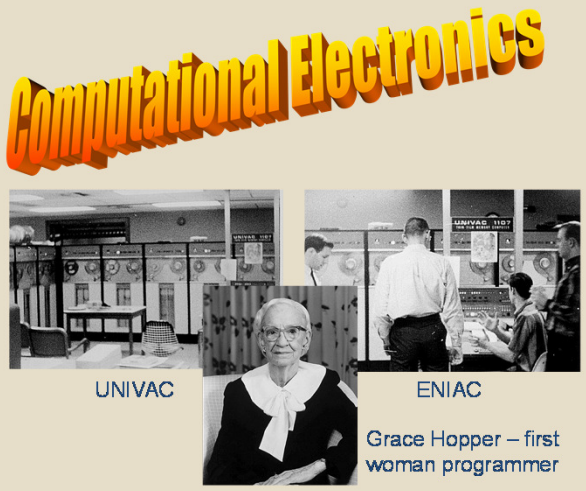
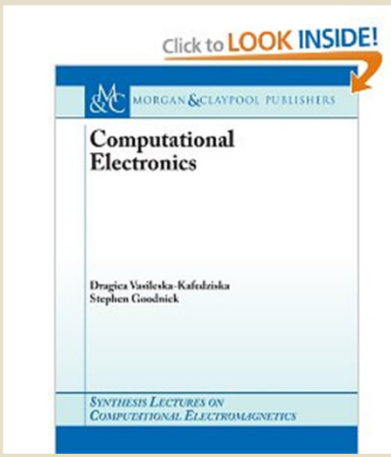
What are the Proper Transport Models at the Nanoscale?

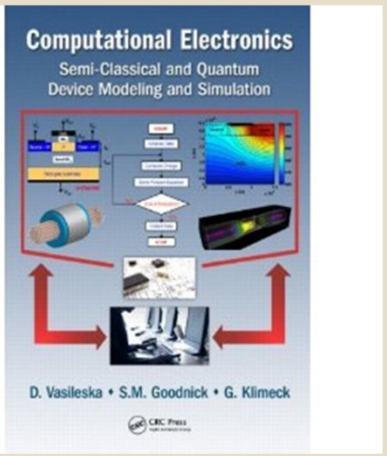
Semiclassical Transport Approaches

Quantum Transport

Atomistic Simulations







Advantages and disadvantages of models

Range of Validity of Different Methods

	$L \ll l_{e-ph}$			$L \sim l_{e-ph}$	$L \gg l_{e-ph}$
	$L < \lambda$	$L < l_{e-e}$	$L \gg l_{e-e}$		
Transport Regime	Quantum	Ballistic	Fluid	Fluid	Diffusive
Scattering	Rare	Rare	e-e (Many), e-ph (Few)		Many
Model:					
Drift-Diffusion					
Hydrodynamic	Quantum Hydrodynamic				
Monte Carlo					
Schrodinger/Green's Functions	Wave				
Applications	Nanowires, Superlattices	Ballistic Transistor	Current IC's	Current IC's	Older IC's

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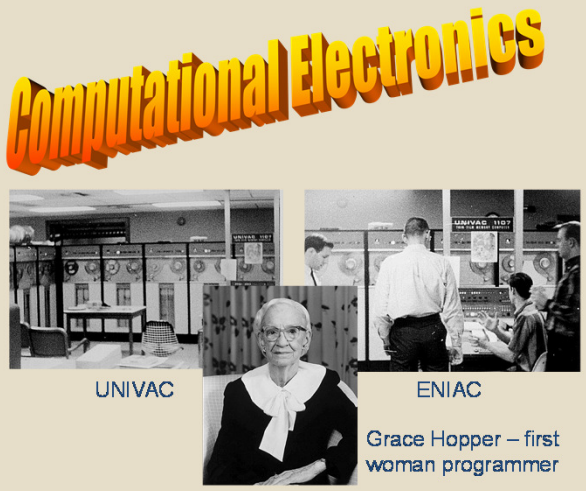
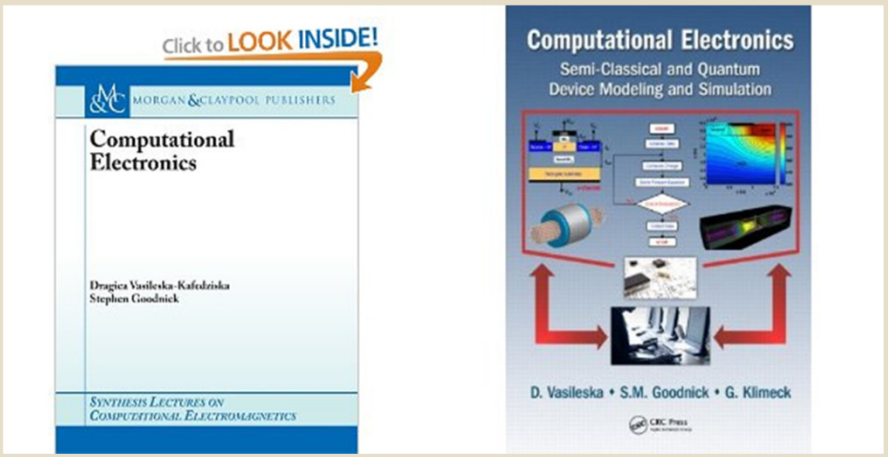




Boltzmann Transport Equation

- In its most general form, the BTE equals to:

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla_r f + (-e)\vec{\varepsilon} \cdot \nabla_p f = \frac{\partial f}{\partial t}\Big|_{coll} =$$

$$= \sum_{i=1}^{N} \sum_{\vec{p}'} [S_i(\vec{p}', \vec{p}) f(\vec{r}, \vec{p}', t) - S_i(\vec{p}, \vec{p}') f(\vec{r}, \vec{p}, t)]$$

- The collision integral on the RHS can be expressed as:

$$RHS = \sum_{\vec{p}'} \sum_{i=1}^{N} [S_i(\vec{p}', \vec{p}) f(\vec{r}, \vec{p}', t)] - f(\vec{r}, \vec{p}, t) \sum_{\vec{p}'} \sum_{i=1}^{N} S_i(\vec{p}, \vec{p}')$$

D. K. Ferry, "*Semiconductors*" (Macmillan, New York, 1991).

Path Integral Solution of the BTE

- The path integral solution of the Boltzmann Transport Equation (BTE), where $L=N\Delta t$ and $t_n=n\Delta t$, is of the form:

$$f_N(t) = \Delta t \sum_{m=0}^{N-1} \underbrace{f_m(p')S_{eff}(p', p+eE(N-m)\Delta t)}_{g_m(p+eE(N-m)\Delta t)} e^{-\Gamma(N-m)\Delta t}$$

K. K. Thornber and Richard P. Feynman, Phys. Rev. B 1, 4099 (1970).

Path Integral Solution of the BTE

- The two-step procedure is then found by using N=1, which means that t=Δt, i.e.:

$$f_1(t) = \Delta t \sum_{p'} \underbrace{f_0(p')S_{eff}(p', p + eE\Delta t)}_{g_0(p + eE\Delta t)} e^{-\Gamma \Delta t}$$

Intermediate function that describes the occupancy of the state (p+eEΔt) at time t=0, which can be changed due to scattering events **(SCATTER)**

+

Integration over a trajectory, i.e.probability that no scattering occurred within time integral Δt **(FREE FLIGHT)**

Rees, H. D., 1969, *J. Phys. Chem. Solids* 30, 643.

Path Integral Solution of the BTE

- Using path integral formulation to the BTE we have shown that one can decompose the solution procedure into two components:
  - **Carrier free-flights** that are interrupted by scattering events

$$\mathrm{k}(t) = \mathrm{k}(0) - e(\mathrm{v} \times \mathrm{B} + \mathrm{E})t / \hbar$$

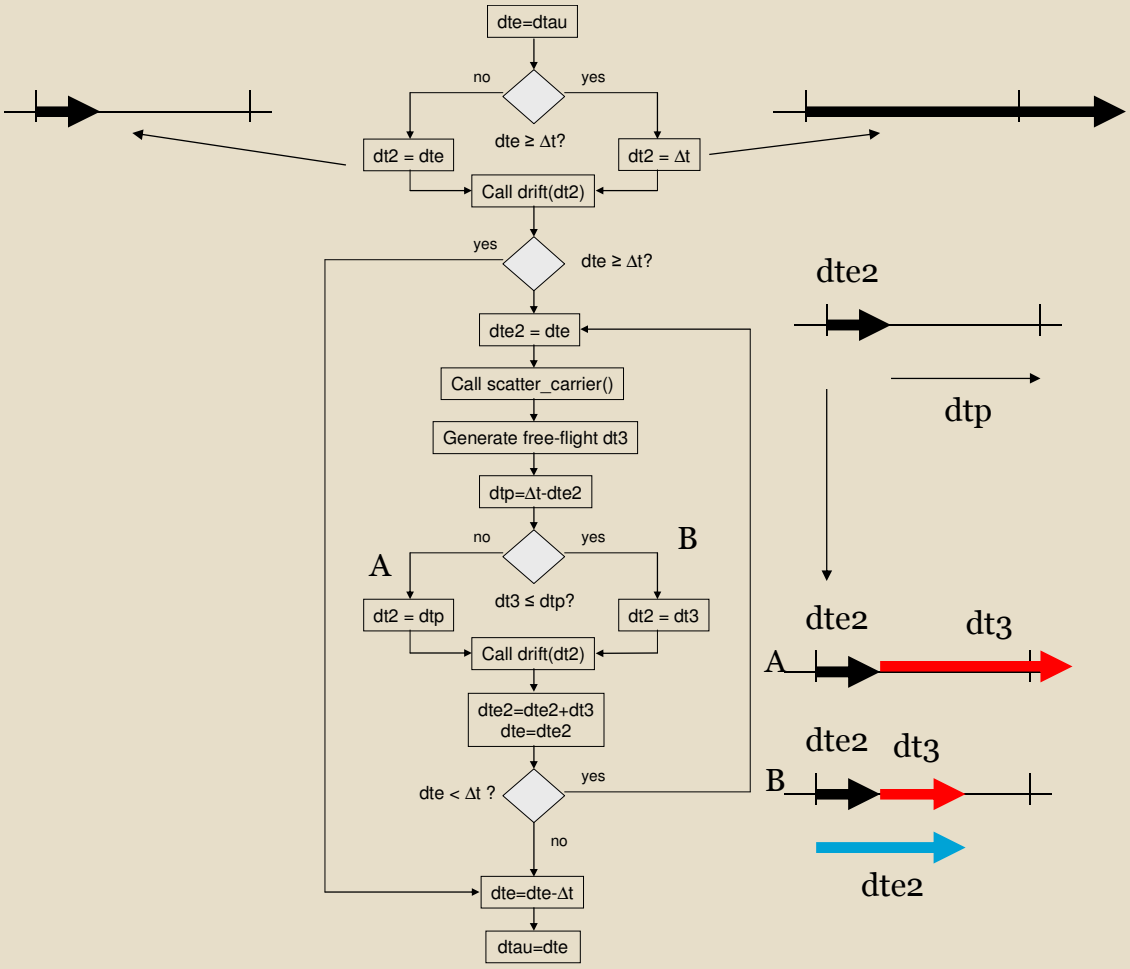
  - **Memory-less scattering events** that change the momentum and the energy of the particle instantaneously

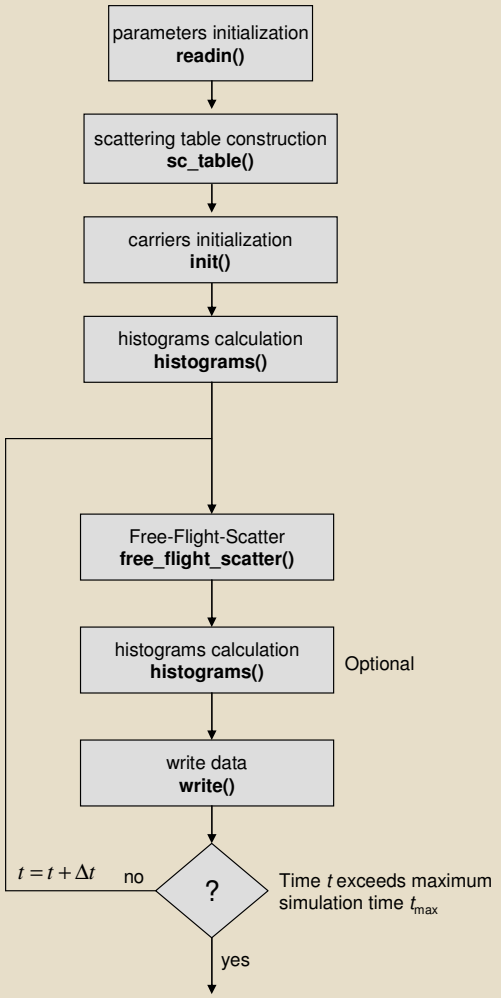
Ways of solving the BTE

- Single particle Monte Carlo Technique
  - Follow single particle for long enough time to collect sufficient statistics
  - Practical for characterization of bulk materials or inversion layers
- Ensemble Monte Carlo Technique
  - MUST BE USED when modeling SEMICONDUCTOR DEVICES to have the complete self-consistency built in

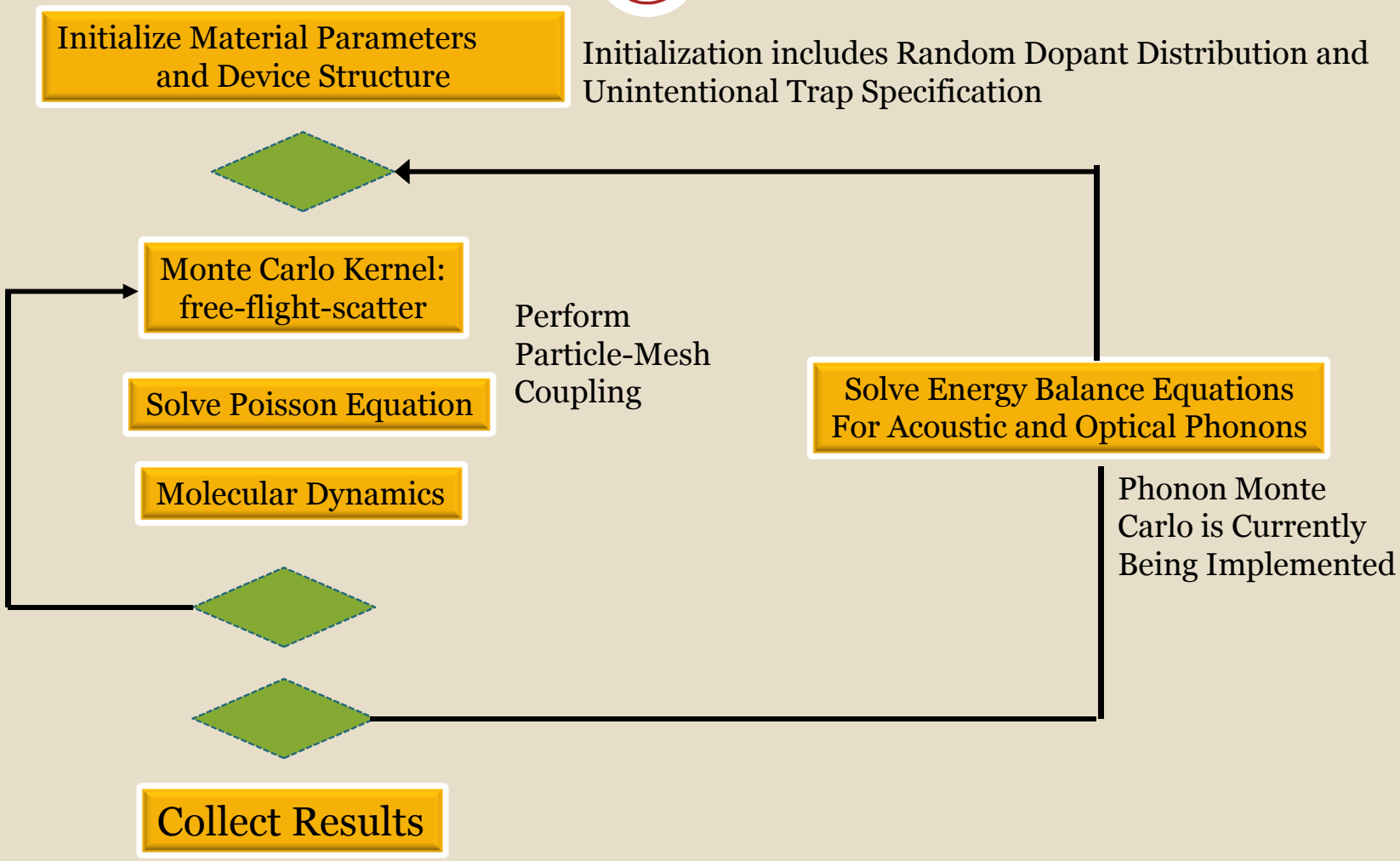
Carlo Jacoboni **and** Lino Reggiani, The Monte Carlo method for the solution of charge transport in semiconductors with applications to covalent materials, Rev. Mod. Phys. 55, 645 - 705 (1983).

Bulk MC Flow-Chart

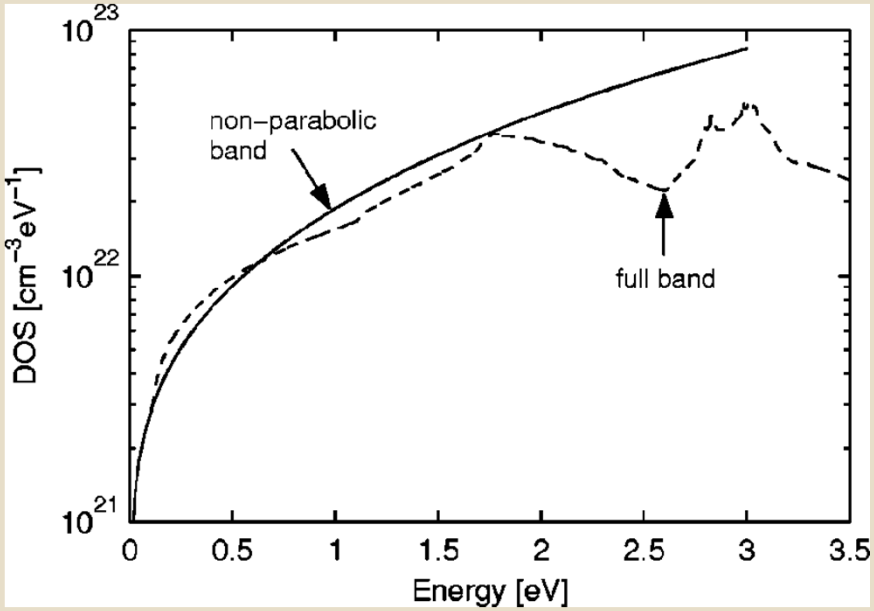


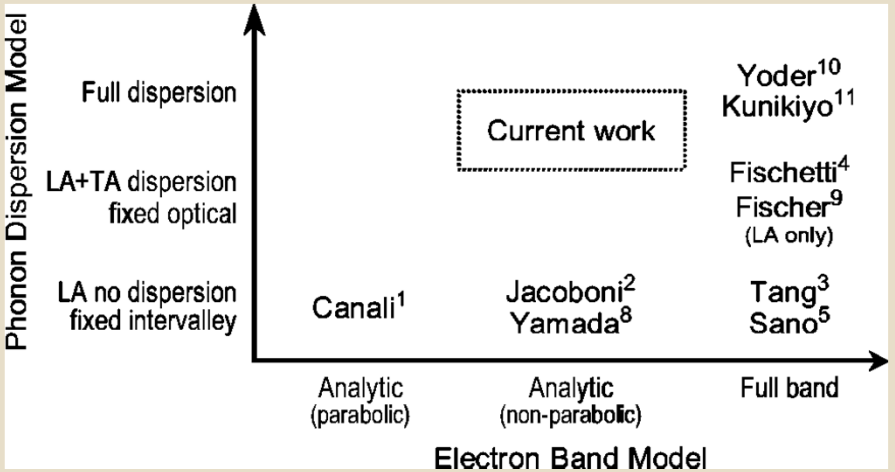


ASU's Particle-Based Device Simulator (Vasileska Group)



The Monte Carlo Method
- Non-parabolicity and Full-Band -



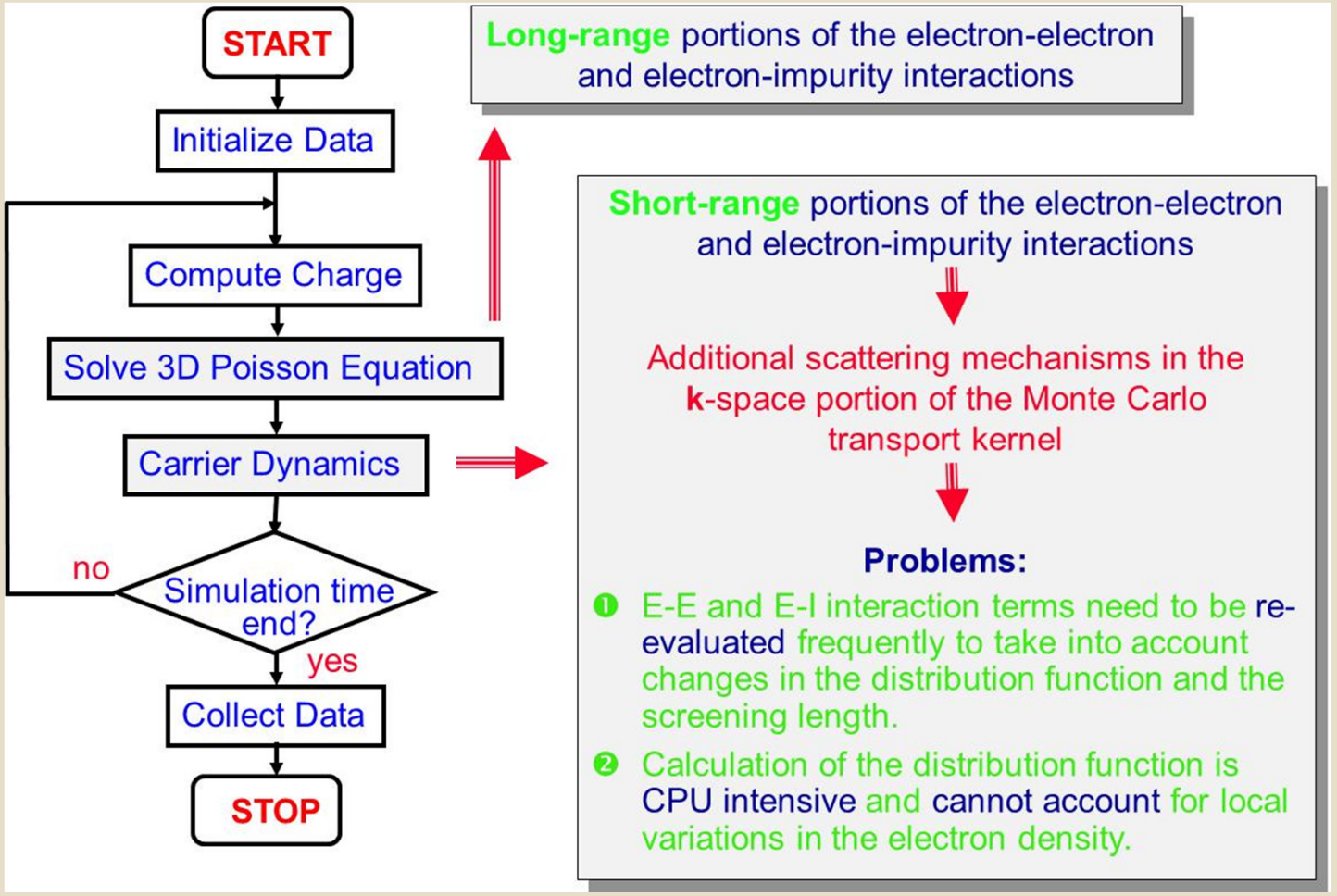


E. Pop, R. W. Dutton and K. E. Goodson, JOURNAL OF APPLIED PHYSICS VOLUME 96, NUMBER 9 1 NOVEMBER 2004

Particle Based Device Simulators

INCORPORATION OF THE SHORT-RANGE COULOMB INTERACTION

K-Space Approach



Real-Space Approach

- Requires 3D device simulator, otherwise the method fails
- There are several variants of this method
  - Corrected Coulomb approach developed by Vasileska and Gross
  - Particle-particle-particle-mesh (p3m) method by Hockney and Eastwood
  - Fast Multipole method

- Corrected Coulomb approach and p3m method are almost equivalent in philosophy, FMM is very different
- Treatment of the short-range Coulomb interactions using any of these three methods accounts for:
  - Binary collisions + plasma (collective) excitations
  - Screening of the Coulomb interactions
  - Scattering from multiple impurities at the same time which is very important at high substrate doping densities

Simulation Methodologies

Method Complexity

P^3M	FMM
$O(N+M\log M)$,	$O(N)$

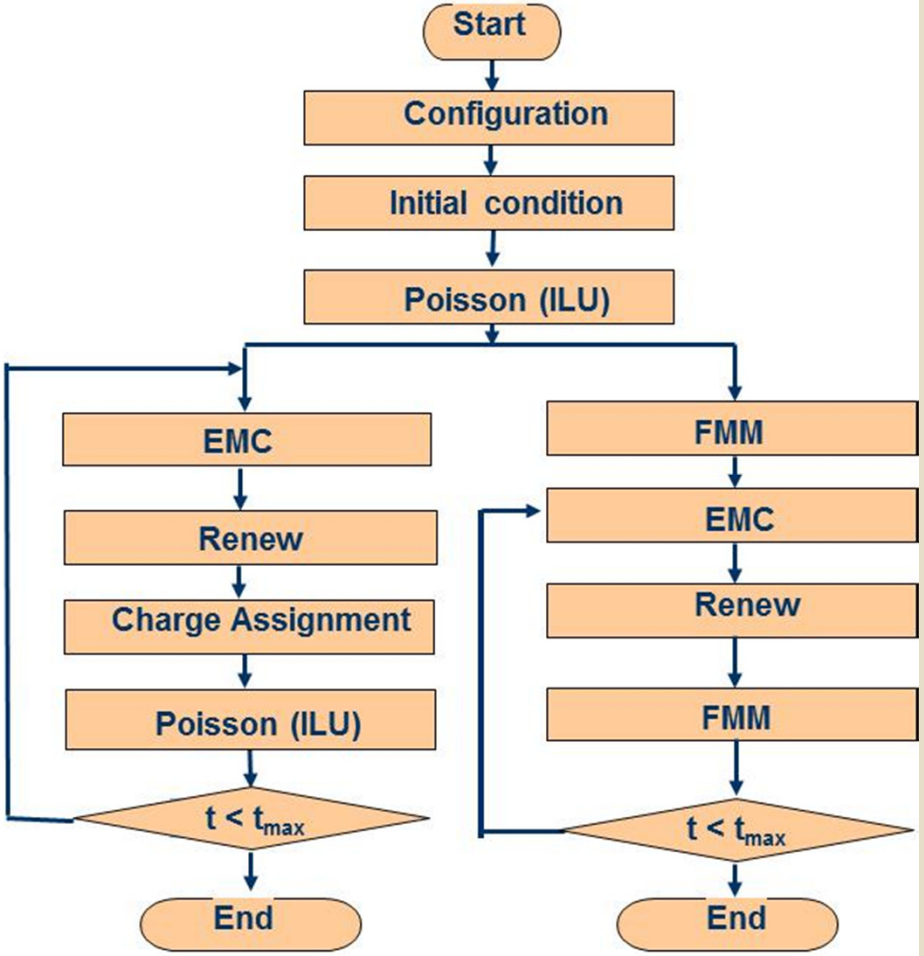
N=Number of particles

M=Number of Mesh Points

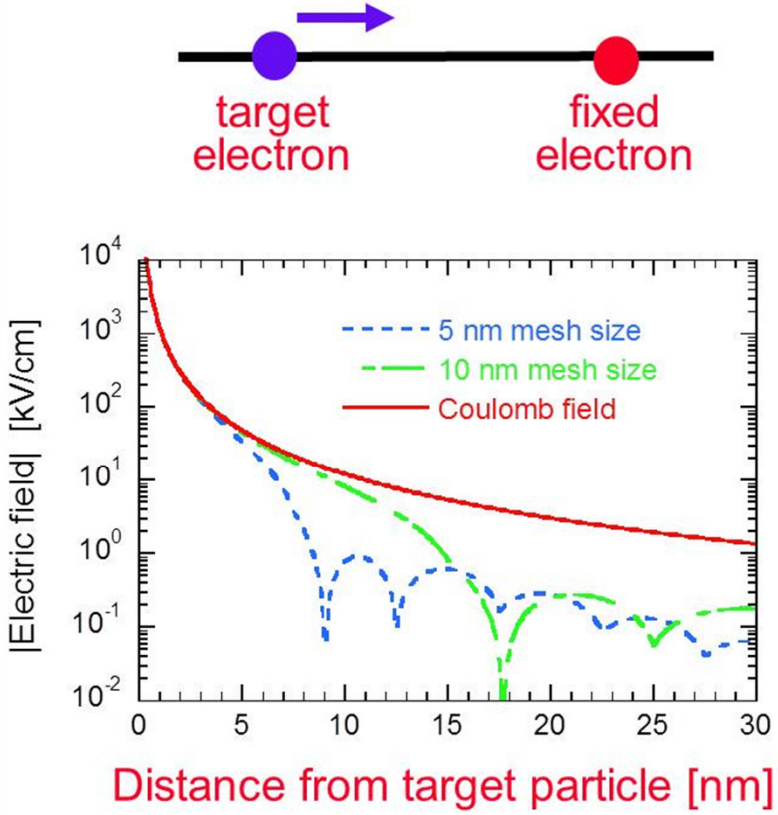
Computation time

Machine: P-4 , 2GHz
Mesh points: 64X24X24
Particles: 690

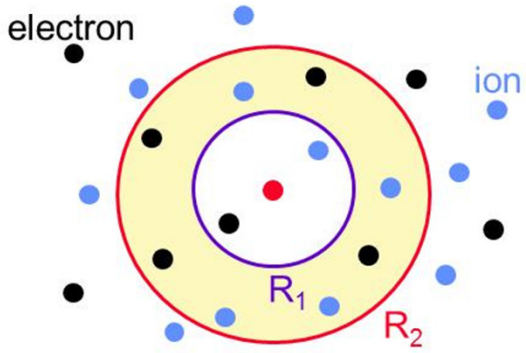
Time for each iteration	
P^3M	FMM
~24 sec	**<1sec**



Corrected Coulomb Approach



- **Double-counting** of the Coulomb force is **eliminated**
- **Limitation:** must use **uniform** mesh spacing
- The generated look-up table gives us information about the **proper cut-off** range

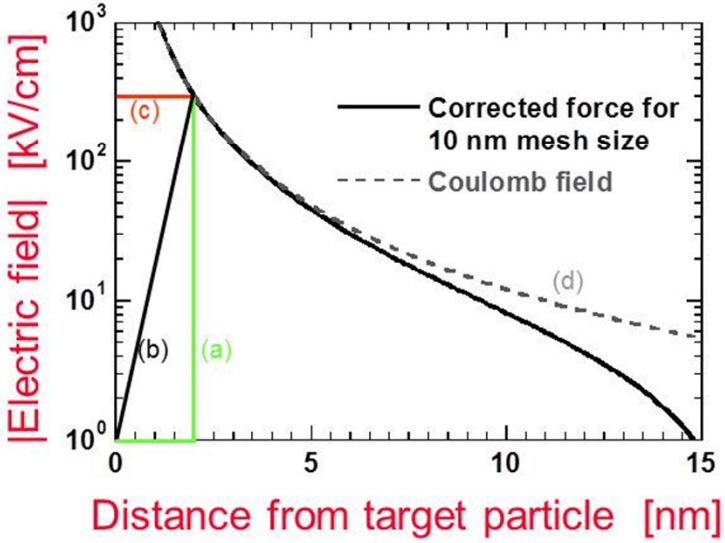


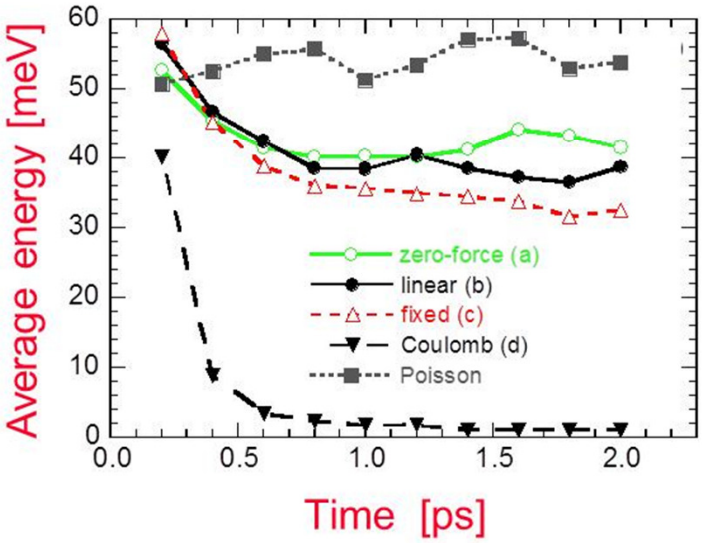
R_2 must be greater than 2× the mesh spacing

W. J. Gross, D. Vasileska and D. K. Ferry, "*IEEE Electron Device Lett*. 20, No. 9, pp.463-465 (1999).

Corrected Coulomb Approach – Cont'd

- The use of the simple Coulomb interaction in the source and drain regions leads to electron trapping which, in turn, prevents the filling of the channel with electrons.
- The carrier trapping can be eliminated through the use of modified short-range Coulomb correction force.

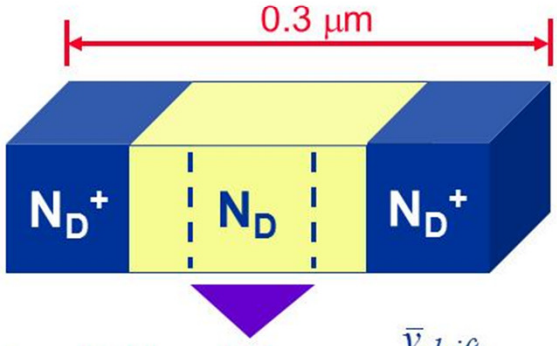




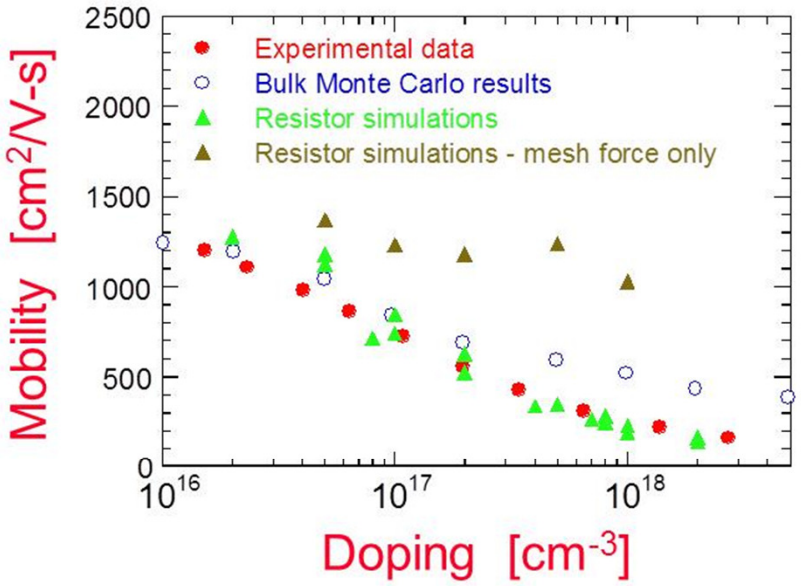
W. J. Gross, D. Vasileska and D. K. Ferry, "*VLSI Design*, Vol. 10, pp. 437-452 (2000).

Corrected Coulomb Approach – Cont'd

- Doping of the N^+- regions: $N_D^+ = 10^{19}$ cm^{-3}.
- Mesh: uniform mesh spacing in all directions equal to 10 nm.
- Cases considered:
  - Mesh force only
  - Mesh force + short-range $e-e$ and $e-i$ interaction terms

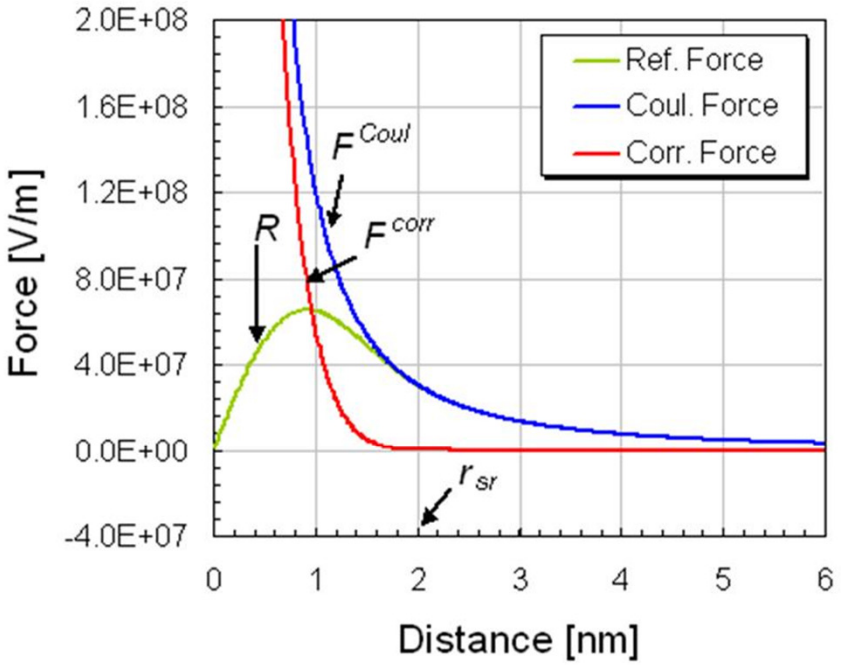


Low-field mobility: $\mu = \dfrac{\bar{v}_{drift}}{E}$



- The **mesh force only** does not give the correct doping dependence of the low-field electron mobility.
- The inclusion of the **short-range interaction terms** gives simulation low-field mobility data in agreement with experimental values.

P3M Approch



$$F_{ij}^{corr} = F_{ij}^{Coul} - R_{ij}$$

R. W. Hockney and J. W. Eastwood, *Computer Simulation Using Particles* (New York, McGraw-Hill, 1981).

Reference force replaces the mesh force and needed to avoid double counting of the short-range force.

The reference force should be equal to the mesh force inside the SR domain and equal to the Coulomb force outside the SR domain.

Roger W. Hockney, James W. Eastwood, *Computer Simulation Using Particles*, Taylor & Francis.

P3M Approach – Cont'd

Smoothing of the total interparticle force between the long-and short-range domains can be thought of as ascribing a finite size to particle *i*.

A sphere with uniformly decreasing density profile, *S*(*r*) is a good choice for smoothing in three dimensions.

$$S(\mathrm{r}) = \begin{cases} \dfrac{48}{\pi r_{sr}^{\ 4}}\left(\dfrac{r_{sr}}{2} - r\right), & r \le r_{sr}/2 \\ 0, & \textit{otherwise}, \end{cases}$$

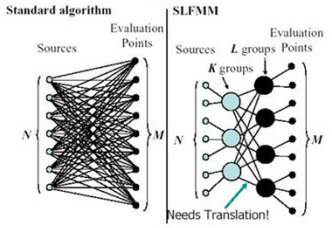
$$\begin{cases} R_{ij}(r) = \dfrac{q_i q_j}{4\pi\varepsilon} \times \dfrac{1}{35 r_{sr}^2}(224\xi - 224\xi^3 + 70\xi^4 + 48\xi^5 - 21\xi^6) & \xi = \dfrac{2r}{r_{sr}} \text{ and } 0 \le r \le r_{sr}/2 \\ R_{ij}(r) = \dfrac{q_i q_j}{4\pi\varepsilon} \times \dfrac{1}{35 r_{sr}^2}\left(\dfrac{12}{\xi^2} - 224 + 896\xi - 840\xi^2 + 224\xi^3 + 70\xi^4 - 48\xi^5 + 7\xi^6\right) & r_{sr}/2 \le r \le r_{sr} \\ R_{ij}(r) = \dfrac{q_i q_j}{4\pi\varepsilon} \times \dfrac{1}{r^2} & r > r_{sr} \end{cases}$$

FMM Approach

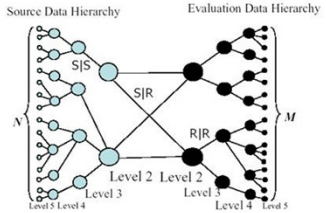
- Introduced by Rokhlin & Greengard in 1987.
- Called one of the 10 most significant advances in computing of the 20th century.
- For a given precision ε, the FMM achieves the evaluation in O(M+N) operations.
- Edelman: "FMM is all about adding functions".

V. Rokhlin and L. Greengard, J. Comp. Phys., Vol. 73, pp. 325-348, 1987.

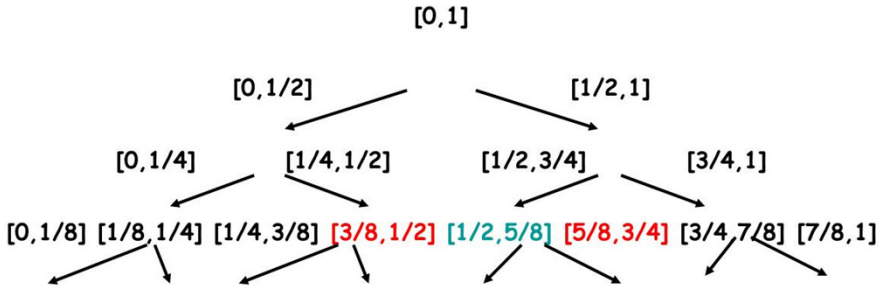
Idea of a Single Level FMM



Idea of Multilevel FMM



- Consider the following binary tree structure induced by a uniform subdivision of the unit interval:



- To approximately evaluate s(x) in the panel [1/2,5/8], we have:

$$s(x) \approx s_{[3/8,1/2]}(x) + s_{[1/2,5/8]}(x) + s_{[5/8,3/4]}(x) + r_{[1/4,3/8]}(x) + r_{[3/4,7/8]}(x) + r_{[7/8,1]}(x) + r_{[0,1/4]}(x)$$

L. Greengard and V. Rokhlin. On the Efficient Implementation of the Fast Multipole Algorithm. Department of Computer Science Research Report 602, Yale University (1988).

FMM Approach

- Introduced by Rokhlin & Greengard in 1987.
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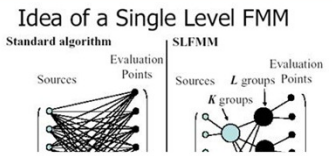


- Consider the following binary tree structure induced by a uniform subdivision of the unit interval:

[0,1]

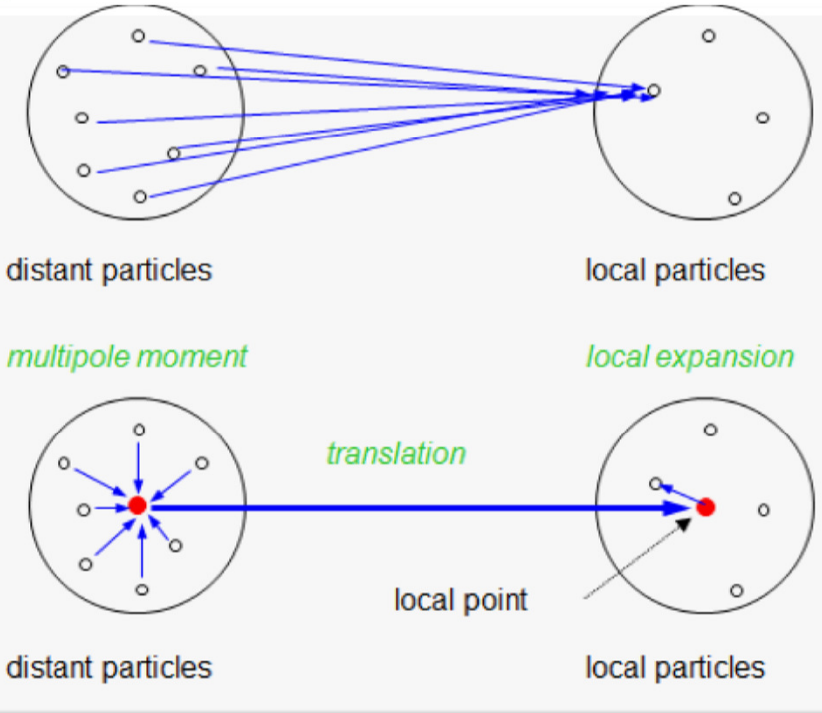
$$\Phi(x) = \sum_{i=1}^{N} \frac{q_i}{|x - y_i|}$$

$$= \sum_{i=1}^{N} q_i \sum_{k=1}^{p} \psi_k(y_i)\phi_k(x)$$

$$= \sum_{k=1}^{p} \phi_k(x) \sum_{i=1}^{N} q_i \psi_k(y_i)$$

$$= \sum_{k=1}^{p} \phi_k(x) A_k$$

L.Greengard and V. Rokhlin, " A Fast Algorithm for Particle Simulations", J. Comp. Phys. V. 135, 280-292 (1997).

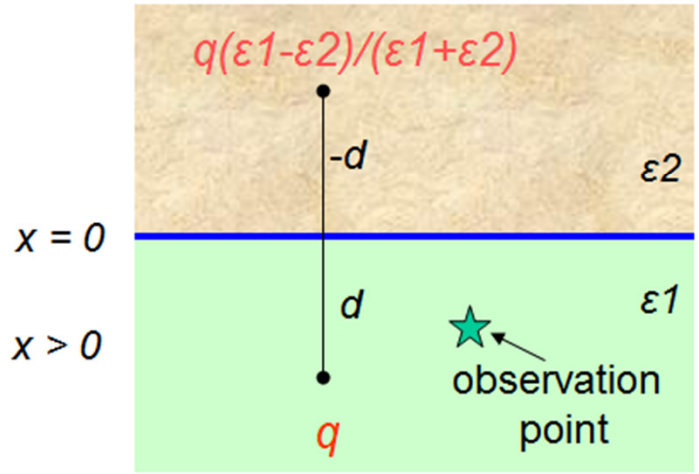


FMM Approach

1. A detailed/comprehensive discussion may be found in:
   L. Greengard and V. Rokhlin, "*A Fast Algorithm for Particle Simulations*", Jour. Comp. Physics, Vol. 135, pp. 280-292, 1997.

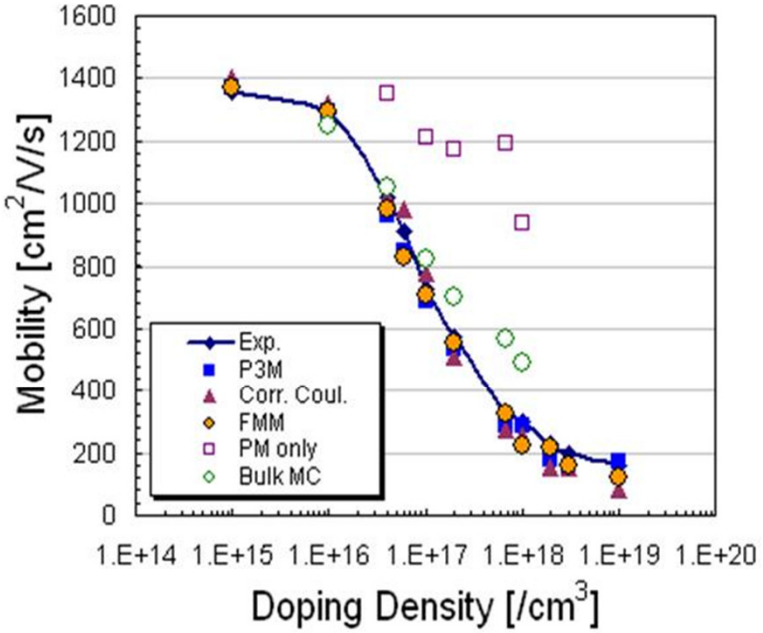
2. Here we present a first-order correction method for the channel charges with the method of images:

   For a point charge q lying in a dielectric e1 distance x = d from the plane boundary between e1 and a second dielectric e2, the given charge plus an image charge q(e1-e2)/(e1+e2) placed at x=-d with all space filled by a dielectric e1 may be used to compute the potential for any point x > 0.



Resistor Simulations

Resistor Simulation:



Method	Time/iteration
P^3M	39 sec
FMM	17 sec

No. of monopole charges: ~22000
Mesh: 40 x 25 x 25

- Uniform mesh (40 x 25 x 25)
- An external field of 1kV/cm was applied to ensure linear region of operation.
- The drift velocity was averaged over 5ps with an interval time of 0.1 ps. The first 1.5 ps data were discarded.

H.R. Khan, D. Vasileska, S.S. Ahmed, C. Ringhofer and C. Heitzinger, *Journal of Computational Electronics*, Vol. 3, Nos. 3-4, pp. 337-340 (2005).

Particle-Based Device Simulators

INCORPORATION OF SELF-HEATING EFFECTS

ASU (Vasileska) Model for Self-Heating Effects

$$\left(\frac{\partial}{\partial t}+v_e(\mathrm{k})\cdot\nabla_r+\frac{e}{\hbar}E(\mathrm{r})\cdot\nabla_k\right)f=\sum_{\mathrm{q}}\left\{W_{e,\mathrm{q}}^{\mathrm{k+q}\to\mathrm{k}}+W_{a,-\mathrm{q}}^{\mathrm{k+q}\to\mathrm{k}}-W_{e,-\mathrm{q}}^{\mathrm{k}\to\mathrm{k+q}}-W_{a,\mathrm{q}}^{\mathrm{k}\to\mathrm{k+q}}\right\}$$

$$\left(\frac{\partial}{\partial t}+v_p(q)\cdot\nabla_r\right)g=\sum_{\mathrm{k}}\left\{W_{e,\mathrm{q}}^{\mathrm{k+q}\to\mathrm{k}}-W_{a,\mathrm{q}}^{\mathrm{k}\to\mathrm{k+q}}\right\}+\left(\frac{\partial g}{\partial t}\right)_{p-p}$$

J. Lai and A. Majumdar, "Concurent thermal and electrical modeling of submicrometer silicon devices", J. Appl. Phys. , Vol. 79, 7353 (1996).

$$C_{LO}\frac{\partial T_{LO}}{\partial t}=\frac{3nk_B}{2}\left(\frac{T_e-T_L}{\tau_{e-LO}}\right)+\frac{nm^*v_d^2}{2\tau_{e-LO}}-C_{LO}\left(\frac{T_{LO}-T_A}{\tau_{LO-A}}\right),$$

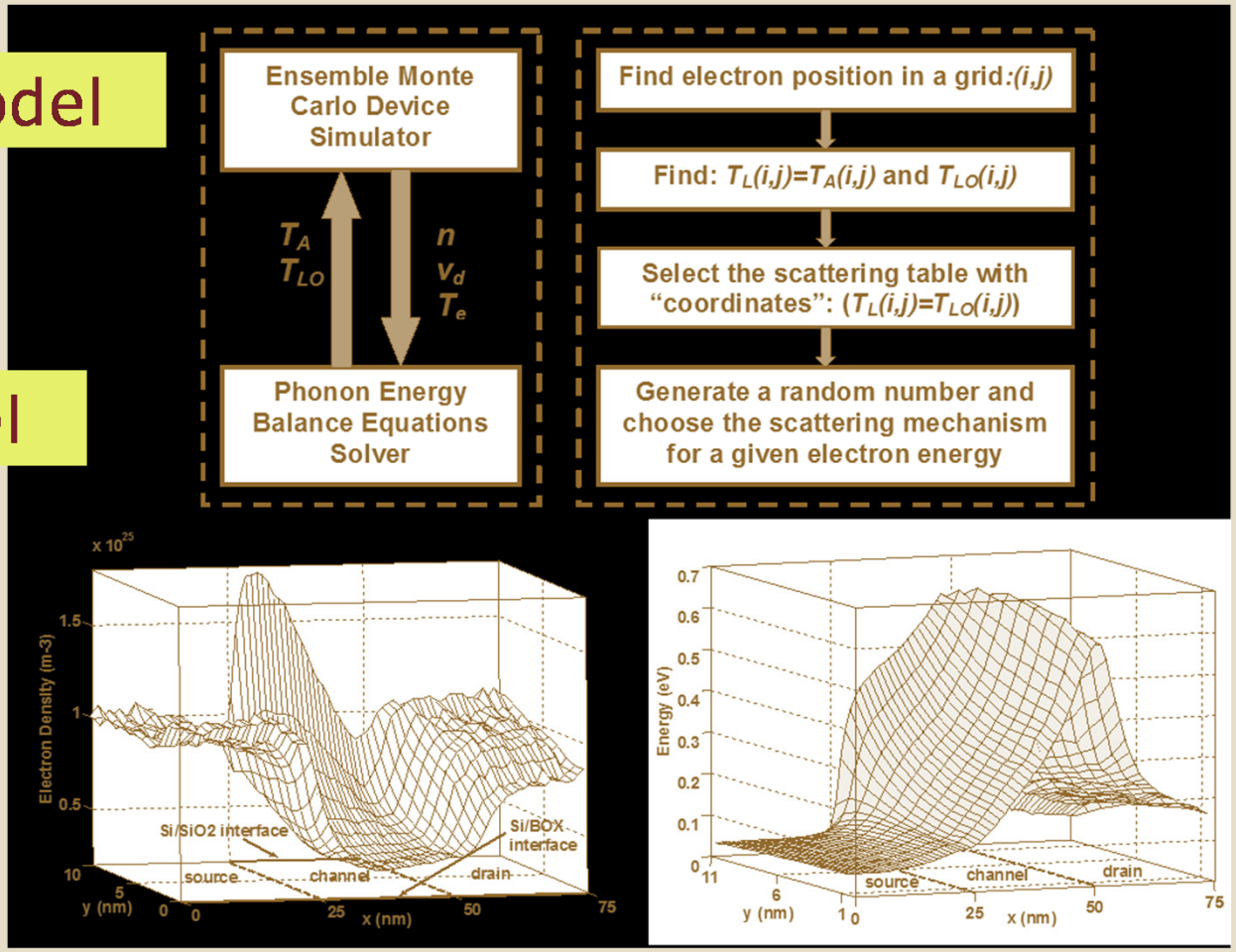
$$C_A\frac{\partial T_A}{\partial t}=\nabla\cdot(k_A\nabla T_A)+C_{LO}\left(\frac{T_{LO}-T_A}{\tau_{LO-A}}\right)+\frac{3nk_B}{2}\left(\frac{T_e-T_L}{\tau_{e-L}}\right).$$

K. Raleva, D. Vasileska, S. M. Goodnick and M. Nedjalkov, IEEE Transactions on Electron Devices, vol. 55, issue 6, pp. 1306-1316, June 2008.

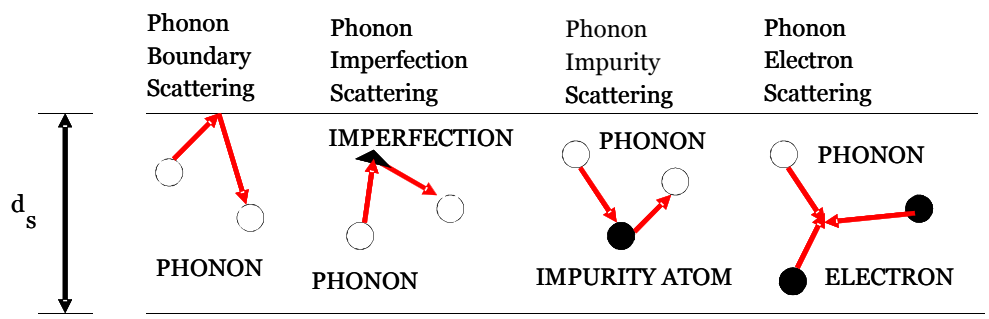
Exchange of variables between the two kernels

Particle Model

Fluid Model



Various factors that affect the thermal conductivity value

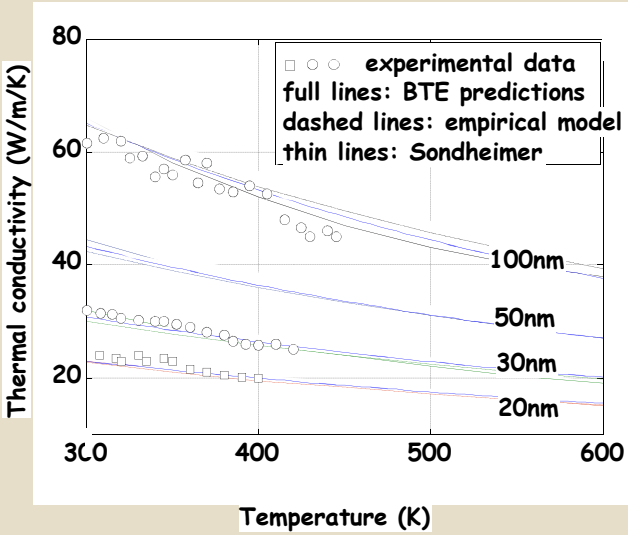


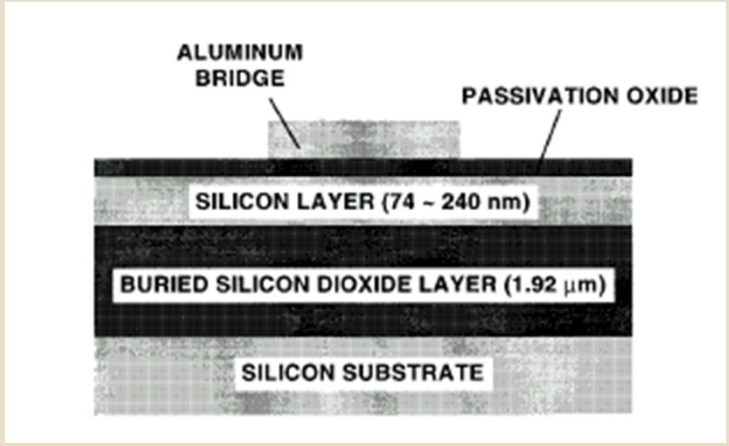
$$\kappa(z) = \kappa_0(T) \int_0^{\pi/2} \sin^3\theta \left\{ 1 - \exp\left(-\frac{a}{2\lambda(T)\cos\theta} \right) \cosh\left(\frac{a-2z}{2\lambda(T)\cos\theta} \right) \right\} d\theta$$

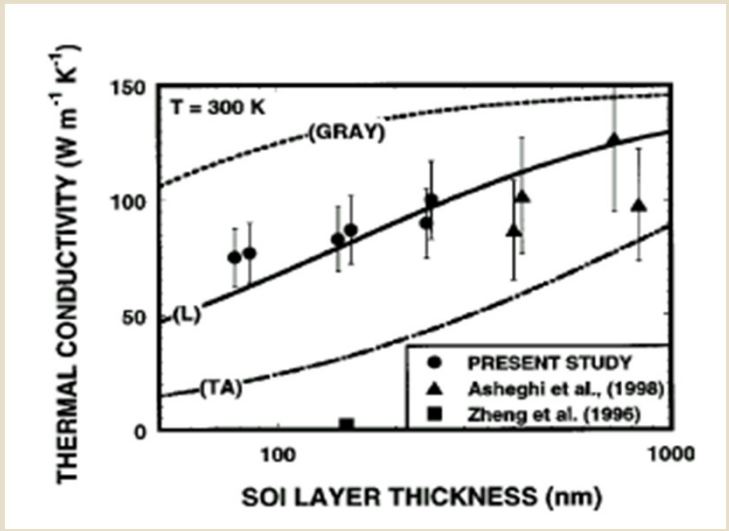
$$\lambda(T) = \lambda_0(300/T)$$

$$\kappa_0(T) = \frac{135}{a + bT + cT^2} \quad \text{W/m/K}$$

Vasileska/Raleva Model for the Thermal Conductivity







Ashegi, Leung, Wong, Goodson, *Appl. Phys. Lett.* 71, 1798 (1997)

Particle-Based Device Simulators

INCORPORATION OF SPIN

Spin-Orbit Effects

- **Rashba SO-coupling**
- **Generating spin polarized currents in nanowires and constrictions**
- **Band structure in 2DEG**
- **Transverse Electron Focalization (TEF) in systems with SO-coupling**
- **Spin accumulation (Spin Hall Effect in ballistic mesoscopic systems)**

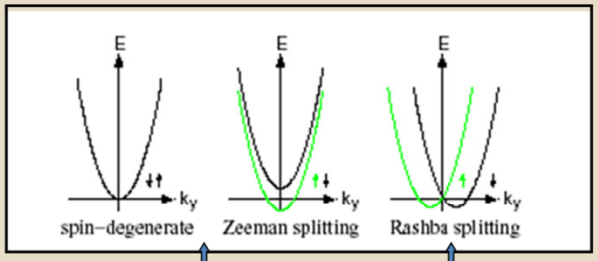
The atomistic effect:

$$M = -\frac{eg}{2mc} S \qquad H = -M \cdot B \qquad B = \frac{1}{c} v \times E$$

$$H = \frac{eg}{2mc} S \cdot B = -\frac{eg}{2mc^2} S \cdot v \times E = \frac{eg}{2m^2 c^2} S \cdot p \times \nabla \phi(r) \quad \frac{1}{2}$$

The Thomas precession effect

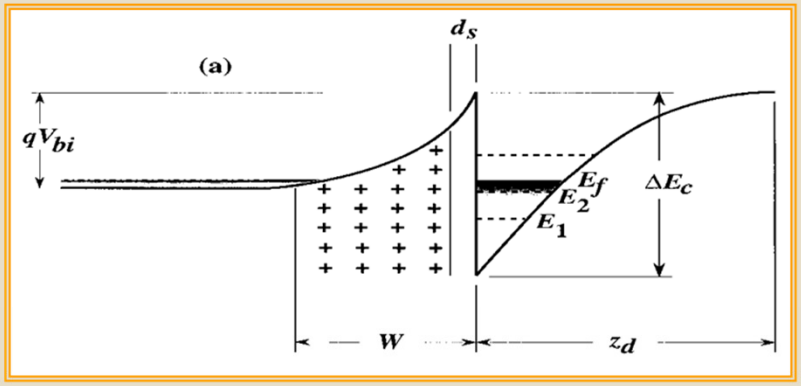
Heterostructures:



$$E_{\pm} = \frac{\hbar^2 k^2}{2m} \pm \mu B \qquad E_{\pm} = \frac{\hbar^2 k^2}{2m} \pm \alpha k$$

The SO-coupling preserves the time reversal symmetry

Rashba Spin-Orbit Coupling



$$H_{SO} = -\frac{e\hbar\boldsymbol{\sigma}\cdot\mathbf{p}\times\mathscr{E}}{4m^2c^2}$$

Rashba spin splitting and Ehrenfest's theorem

R. Winkler*

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Physica E 22 (2004) 450–454

material

$$H_{SO} = \frac{\alpha}{\hbar}(p_y\sigma_x - p_x\sigma_y)$$

Can be controlled with external gates

	α
GaAs/AlGaAs	0.5–1 meV nm
InSb/InAlSb	5–10 meV nm

Nitta *et al*. PRL **78** (1997)

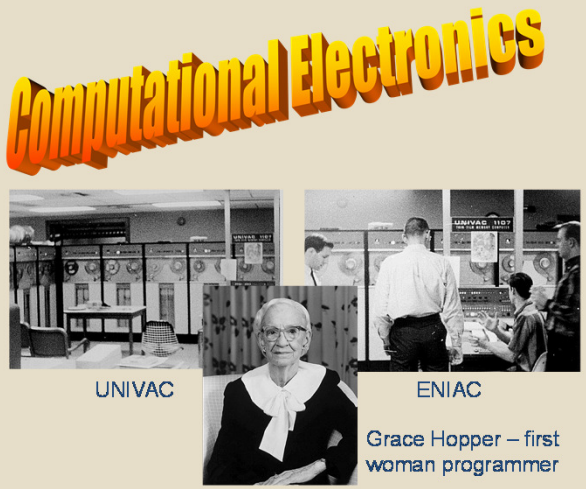
Miller *et al* PRL **90** 076807 (2003)

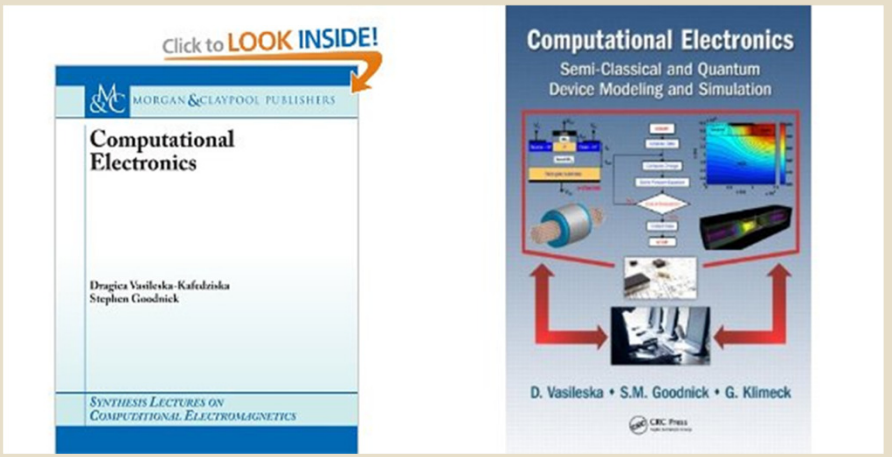
What are the Proper Transport Models at the Nanoscale?

Semiclassical Transport Approaches

Quantum Transport

Atomistic Simulations





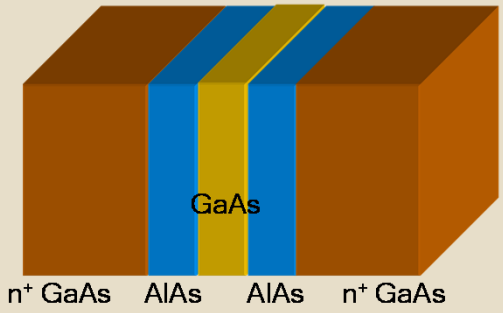
What do we cover in this section?

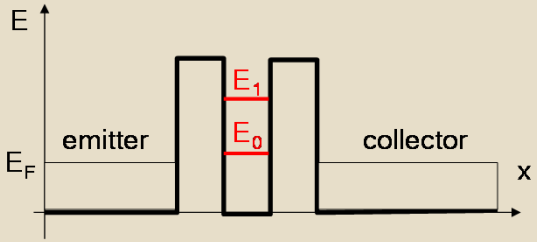
- Quantum Transport
  - Solution of the Schrodinger Equation Using Usuki Method
  - Green's Functions
    - Recursive Green's Function Approach
    - Contact Block Reduction Method and its applications

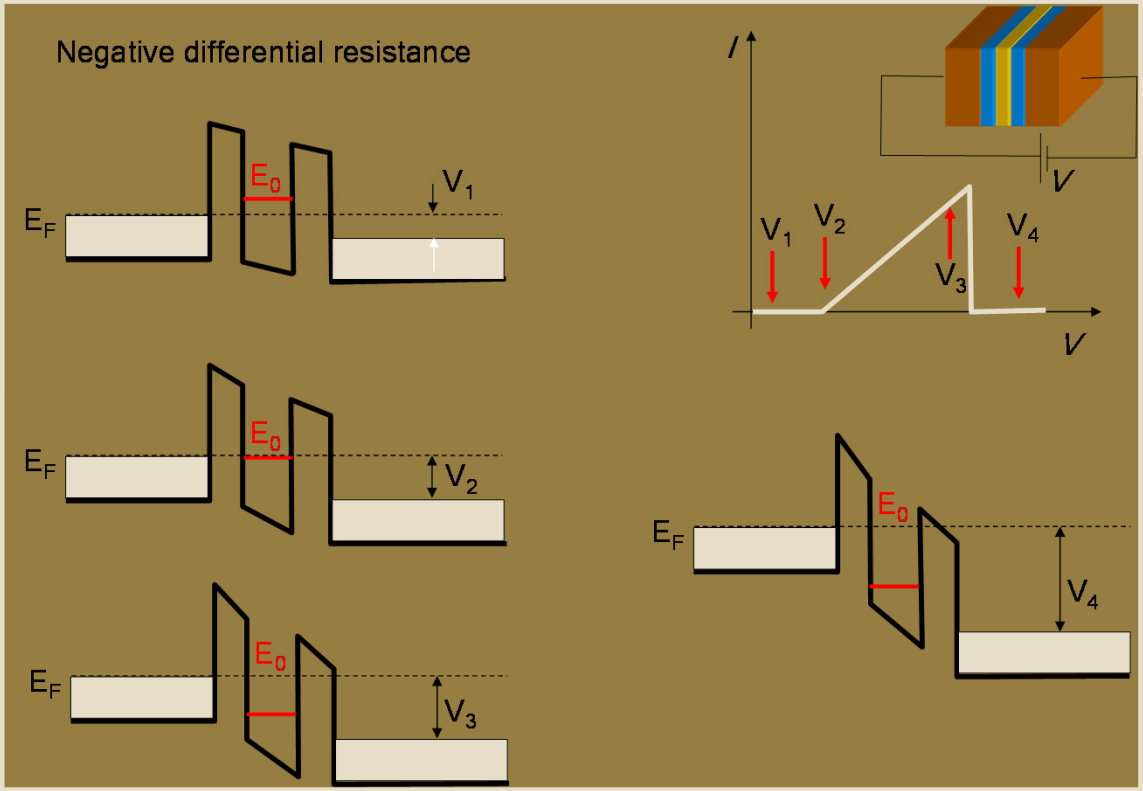
Quantum Transport

USUKI METHOD

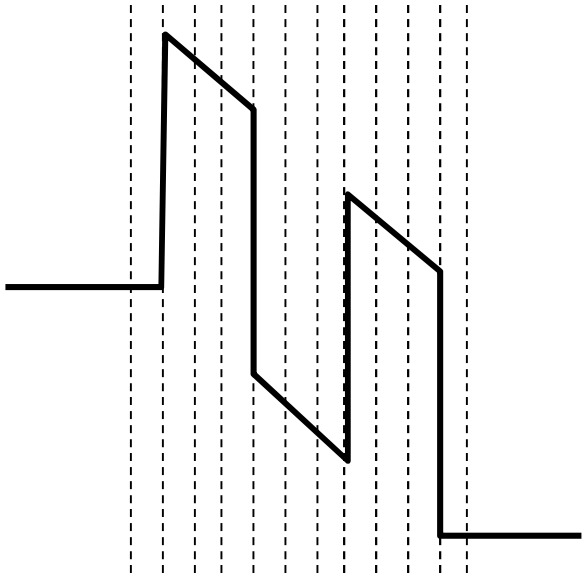
Transfer Matrix Approach on the Example of RTD





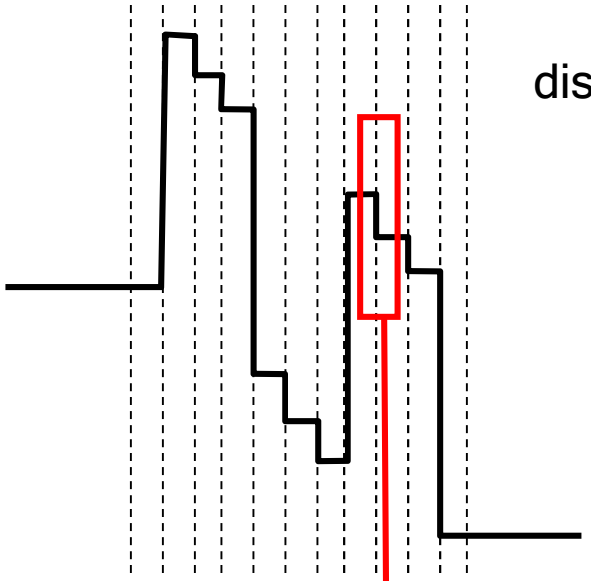


How to calculate the transfer matrix T?



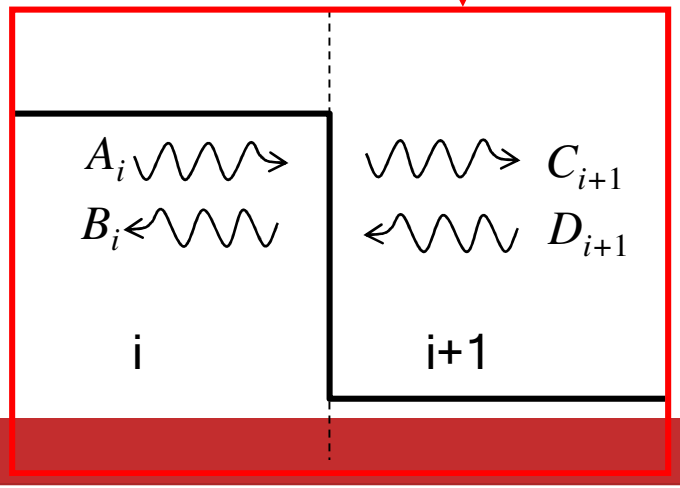
divide the active region into N slices

How to calculate the transfer matrix T?



discretize the potential

divide the active region into N slices



consider a boundary between slices i and i+1:

write down solutions for slices i and i+1

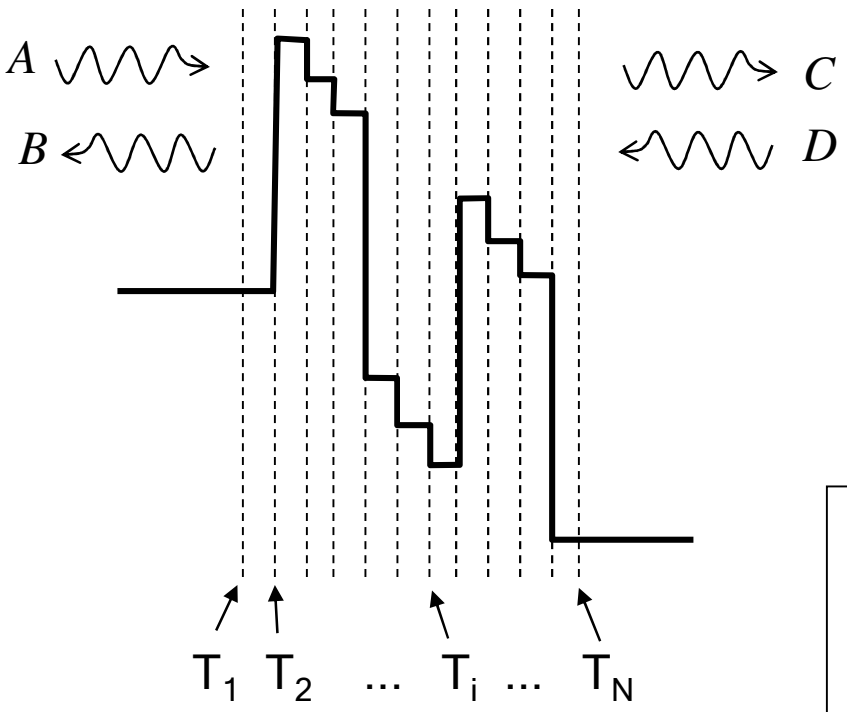
$$\psi^{\mathrm{i}}(z) = A_i e^{ik_z^i z} + B_i e^{-ik_z^i z}$$
$$\psi^{\mathrm{i+1}}(z) = C_{i+1} e^{ik_z^{i+1} z} + D_{i+1} e^{-ik_z^{i+1} z}$$

use the continuity conditions

$$\psi^{\mathrm{i}}(z_i) = \psi^{\mathrm{i+1}}(z_i)$$
$$\frac{\partial}{\partial z}\psi^{\mathrm{i}}(z_i) = \frac{\partial}{\partial z}\psi^{\mathrm{i+1}}(z_i)$$

to calculate transfer matrix T_i between slices i and i+1

$$\begin{pmatrix} C_{i+1} \\ D_{i+1} \end{pmatrix} = T_i \begin{pmatrix} A_i \\ B_i \end{pmatrix}$$



total transfer matrix:

$$\begin{pmatrix} C \\ D \end{pmatrix} = T \begin{pmatrix} A \\ B \end{pmatrix}$$

$$T = T_N T_{N-1} \ldots T_i \ldots T_2 T_1$$

$$T = \begin{pmatrix} 1/t^* & -r^*/t^* \\ -r/t & 1/t \end{pmatrix}$$

Transfer matrix is numerically unstable

Scattering matrix S
is numerically stable:

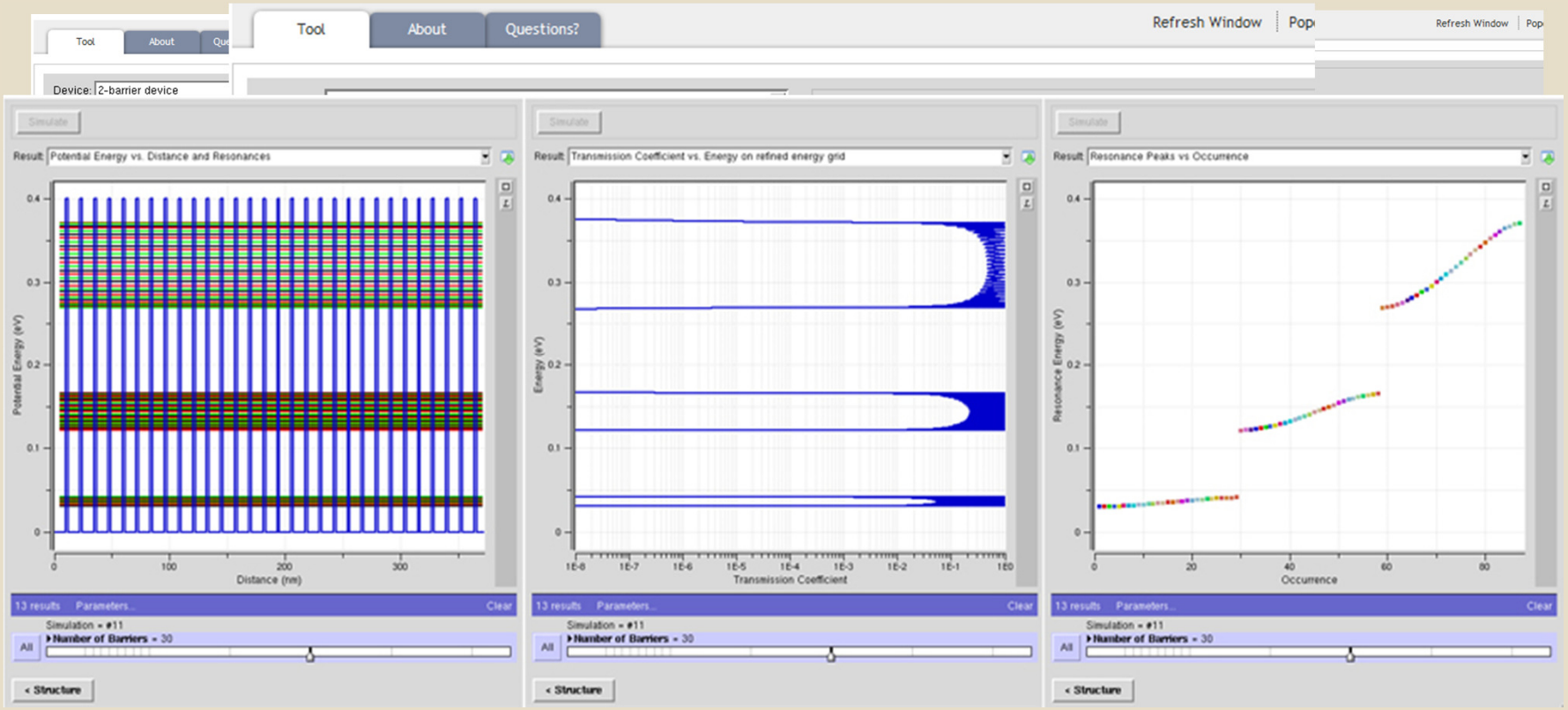
$$\begin{pmatrix} C \\ B \end{pmatrix} = S \begin{pmatrix} A \\ D \end{pmatrix}$$

outgoing states

incoming states

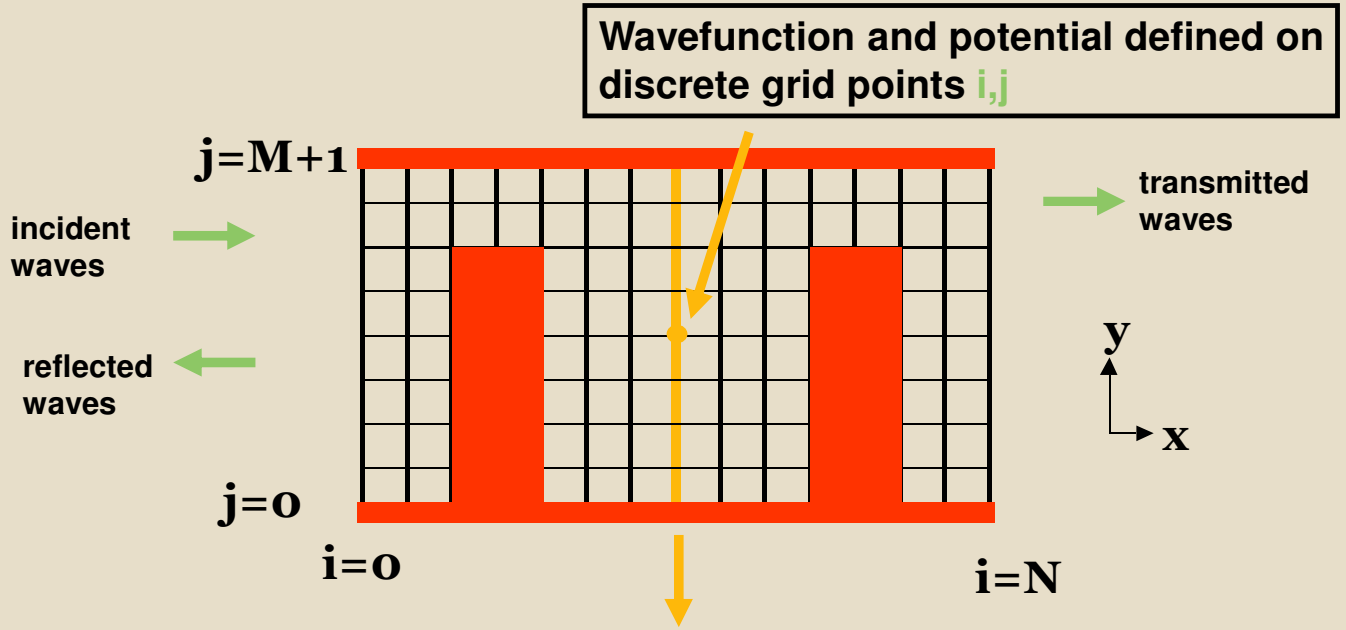
Exercise for PCPBT

- From one well, to two wells to 5 wells (energy bands formation)



Usuki Method Explained

Calculate conductance using finite difference grid



Grid spacing: $a << \lambda_F$

Slides Courtesy of Richard Akis, ASU.

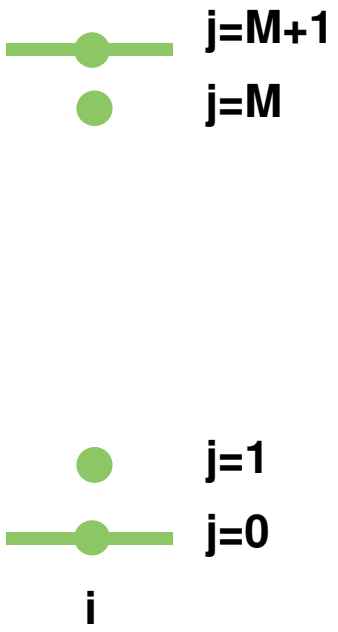
Obtaining transfer matrices from the discrete SE

apply Dirichlet boundary conditions on upper and lower boundary:

$$\psi_{i,j=0} = \psi_{i,j=M+1} = 0$$

Wave function on ith slice can be expressed as a vector

$$\vec{\psi}_i = \begin{bmatrix} \psi_{i,M} \\ \psi_{i,M-1} \\ \cdot \\ \cdot \\ \cdot \\ \psi_{i,1} \end{bmatrix}$$



Discrete SE now becomes a matrix equation relating the wavefunction on adjacent slices:

(1b) $$\mathbf{H_{0i}}\vec{\psi}_i - t\vec{\psi}_{i+1} - t\vec{\psi}_{i-1} = E\vec{\psi}_i$$

where: $$\mathbf{H_{0i}} = \begin{bmatrix} (V_{i,M}+4t) & -t & 0 & \cdots & & & \\ -t & (V_{i,M}+4t) & -t & \cdots & & & \\ & & & \cdots & & & \\ & & & \cdots & -t & (V_{i,2}+4t) & -t \\ & & & \cdots & 0 & -t & (V_{i,1}+4t) \end{bmatrix}$$

(1b) can be rewritten as: $\vec{\psi}_{i+1} = \left(\frac{\mathbf{H_{0i}} - E}{t} \right) \vec{\psi}_i - \vec{\psi}_{i-1}$

Combining this with the trivial equation $\vec{\psi}_i = \vec{\psi}_i$ **one obtains:**

(2) $$\begin{bmatrix} \vec{\psi}_i \\ \vec{\psi}_{i+1} \end{bmatrix} = \mathbf{T_i} \begin{bmatrix} \vec{\psi}_{i-1} \\ \vec{\psi}_i \end{bmatrix}$$

where $$\mathbf{T_i} = \begin{bmatrix} 0 & -\mathbf{I} \\ -\mathbf{I} & \left(\frac{\mathbf{H_{0i}} - E}{t} \right) \end{bmatrix}$$

Is the transfer matrix relating adjacent slices

Modification for a perpendicular magnetic field (0,0,B) :

$$\mathbf{T_i} = \begin{bmatrix} 0 & -\mathbf{I} \\ -\mathbf{P}^2 & \left(\frac{\mathbf{P}(\mathbf{H_{0i}} - E)}{t} \right) \end{bmatrix}$$

B enters into phase factors

$$P_{i,j} = e^{i 2\pi \beta j} \delta_{i,j},$$

important quantity:

flux per unit cell →

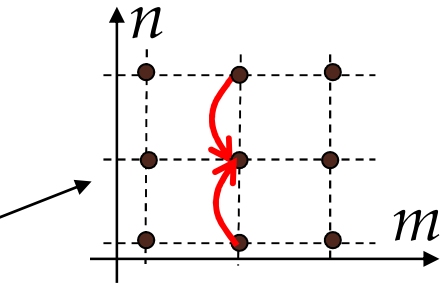
$$\beta = \frac{Ba^2}{h/e} = \varphi / \varphi_0$$

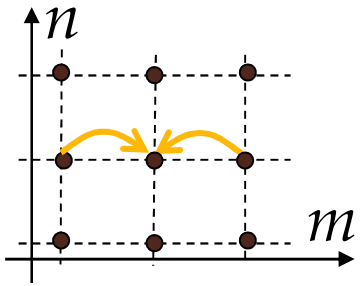
An aside – how the Peierl's substitution appears in a tight-binding Hamiltonian

$$\mathbf{k} \rightarrow -i\nabla - e\mathbf{A}/\hbar, \qquad \Psi \rightarrow \Psi \exp\left(-i\,2\pi\,\mathbf{A}\cdot\mathbf{r}/\phi_0\right),$$

$$H = \sum_{m,n} |m,n\rangle(\varepsilon_0 + V_{mn})\langle m,n| + t|m,n\rangle(\langle m,n+1| + \langle m,n-1|) +$$
$$+ t|m,n\rangle\left(e^{iBa^2n/\hbar}\langle m+1,n| + e^{-iBa^2n/\hbar}\langle m-1,n|\right)$$

magnetic field (Peierls substitution)





Solving the eigenvalue problem: $\mathbf{T}_1\begin{bmatrix}\vec{\psi}_1\\ \vec{\psi}_0\end{bmatrix}=\lambda\begin{bmatrix}\vec{\psi}_1\\ \vec{\psi}_0\end{bmatrix}$ **yields the modes on the left side of the system**

Mode eigenvectors have the generic form: $\begin{bmatrix}\vec{u}_m(\pm)\\ \lambda_m(\pm)\vec{u}_m(\pm)\end{bmatrix}$ ← **redundant**

There will be M modes that propagates to the right (+) with eigenvalues:

$\lambda_m(+)=e^{ik_m a}, m=1,\cdots,q$ **propagating**

$\lambda_m(+)=e^{-\kappa_m a}, m=q+1,\cdots,M$ **evanescent**

There will be M modes that propagates to the left (+) with eigenvalues:

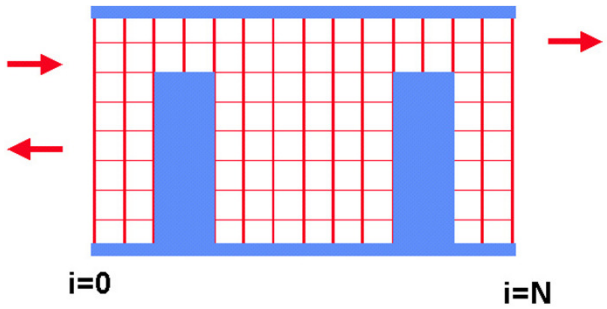
$\lambda_m(-)=e^{-ik_m a}, m=1,\cdots,q$ **propagating**

$\lambda_m(-)=e^{\kappa_m a}, m=q+1,\cdots,M$ **evanescent**

defining $\mathbf{U}_\pm=\begin{bmatrix}\vec{u}_1(\pm) & \cdots & \vec{u}_m(\pm)\end{bmatrix}$ **and** $\lambda_\pm=diag\begin{bmatrix}\lambda_1(\pm) & \cdots & \lambda_m(\pm)\end{bmatrix}$

Complete matrix of eigenvectors: $\mathbf{U}_{\mathbf{tot}}=\begin{bmatrix}\mathbf{U}_+ & \mathbf{U}_-\\ \lambda_+\mathbf{U}_+ & \lambda_-\mathbf{U}_-\end{bmatrix}$

Transfer matrix equation for translation across entire system



Transmission matrix

Unit matrix waves incident from left have unit amplitude

$$\begin{bmatrix} \mathbf{t} \\ \mathbf{0} \end{bmatrix} = \mathbf{U}_{tot}^{-1} \mathbf{T}_{N-1} \mathbf{T}_{N-2} \cdots \mathbf{T}_1 \mathbf{U}_{tot} \begin{bmatrix} \mathbf{I} \\ \mathbf{r} \end{bmatrix}$$

reflection matrix

Zero matrix no waves incident from right

Converts back to mode basis

Converts from mode basis to site basis

Recall: $$G = \frac{2e^2}{h} \sum_{m,n} \frac{v_n}{v_m} \left| t_{n,m} \right|^2$$ → In general, the velocities must be determined numerically

Variation on the cascading scattering matrix technique method
Usuki et al. Phys. Rev. B 52, 8244 (1995)

Boundary condition- waves of unit amplitude incident from right

$$\longrightarrow \quad C_1^{(0,0)} = I, C_2^{(0,0)} = 0$$

Iteration scheme for interior slices

$$\begin{bmatrix} C_1^{(i+1,0)} & C_2^{(i+1,0)} \\ 0 & I \end{bmatrix} = T_i \begin{bmatrix} C_1^{(i,0)} & C_2^{(i,0)} \\ 0 & I \end{bmatrix} P_i$$

$$P_i = \begin{bmatrix} I & 0 \\ P_{i1} & P_{i2} \end{bmatrix},$$

$$P_{i1} = -P_{i2} T_{i21} C_1^{(i,0)},$$

$$P_{i2} = [T_{i21} C_2^{(i,0)} + T_{i22}]^{-1}$$

plays an analogous role to Dyson's equation in Recursive Greens Function approach

Final transmission matrix for entire structure is given by

$$t = -\left(U^+ \lambda^+\right)^{-1} \left[C_1^{N+1} - U^+ \left(U^+ \lambda^+\right)^{-1}\right]^{-1}$$

A similar iteration gives the reflection matrix

After the transmission problem has been solved, the wave function can be reconstructed

It can be shown that:

$$\mathbf{P}_{N2} = \boldsymbol{\psi}_N = \left[\vec{\psi}_{N,1} \quad \cdots \quad \vec{\psi}_{N,k} \quad \cdots \quad \vec{\psi}_{N,M}\right]$$

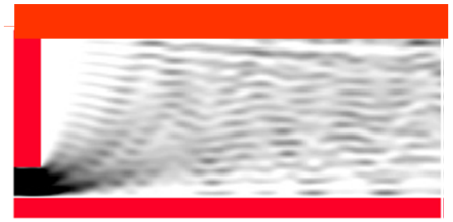
wave function on column N resulting from the *k*th mode

One can then iterate backwards through the structure:

$$\boldsymbol{\psi}_i = \mathbf{P}_{i1} + \mathbf{P}_{i2}\boldsymbol{\psi}_{i+1}$$

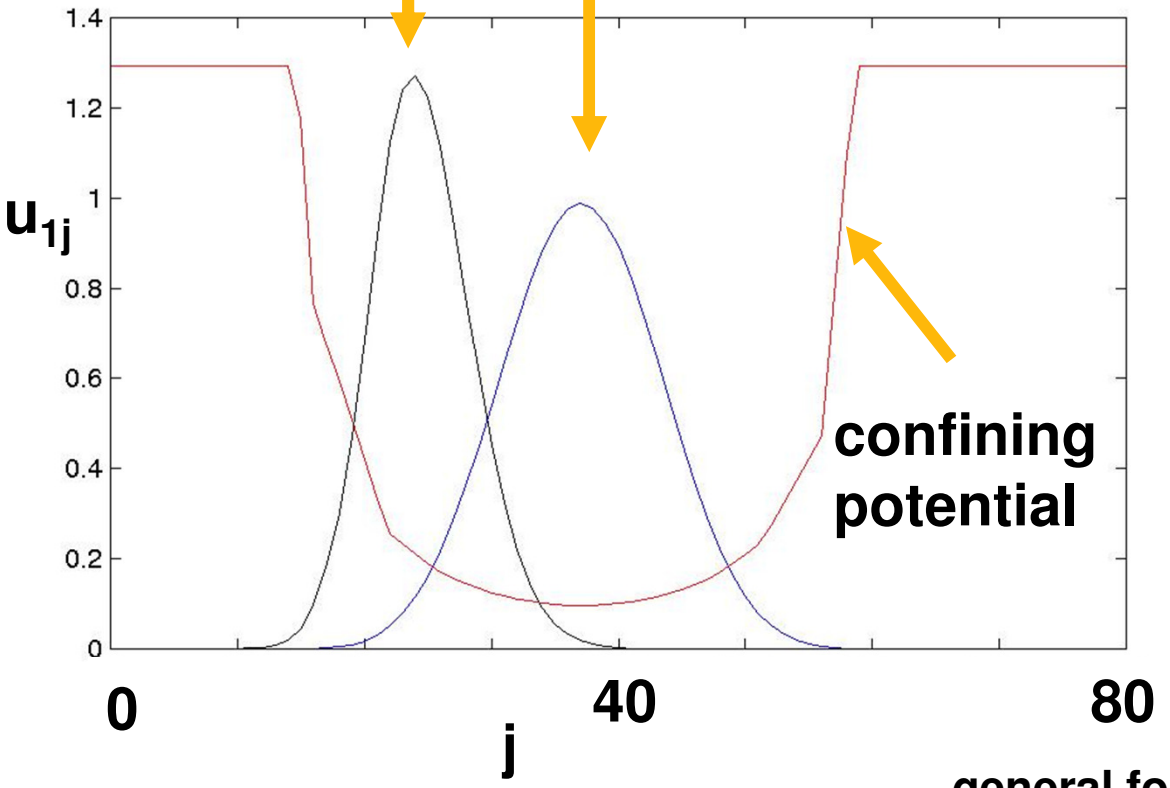
The electron density at each point is then given by:

$$n(x,y) = n(i,j) = \sum_{k=1}^{q} \left|\psi_{ijk}\right|^2$$



First propagating mode for an irregular potential

$\vec{u}_1(+)$ for B=0.7 T $\vec{u}_1(+)$ for B=0 T



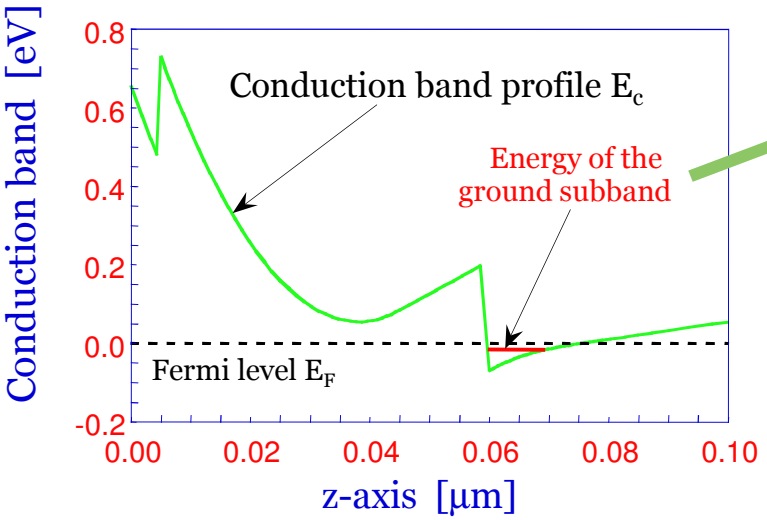
$$\vec{u}_n \equiv \varphi_n(y)$$

Mode functions no longer simple sine functions

$$v_m = \frac{e}{h}\sum_j 2t\,\sin(2k_m - 2\pi\beta\, j)\,u_{mj}^2$$

general formula for velocity of mode m obtained by taking the expectation value of the velocity operator with respect to the basis vector.

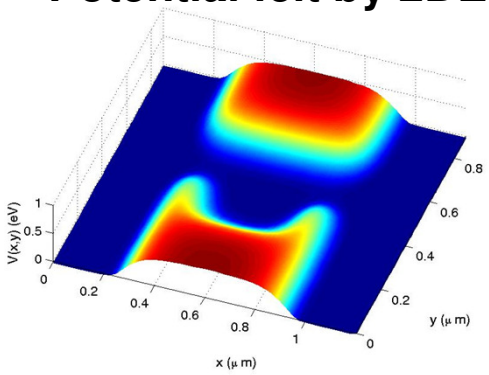
Example – Quantum Dot Conductance as a Function of Gate voltage



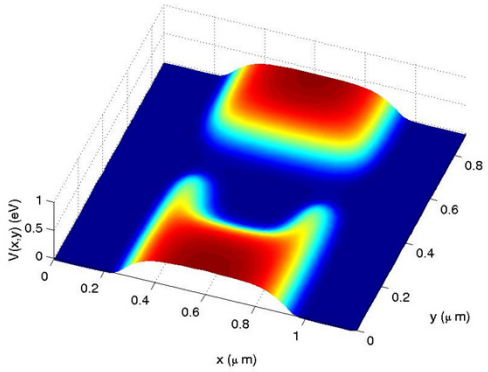
Simulation gives comparable 2D electron density to that measured experimentally

$$N = \frac{\hbar^2}{2m^*}(E_F^{3D} - E_0) \sim 4\times10^{11}\ cm^{-2}$$

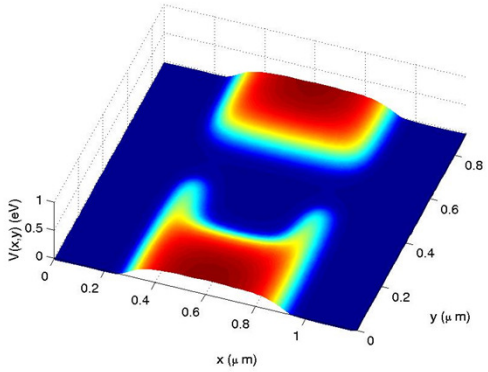
Potential felt by 2DEG- maximum of electron distribution ~7nm below interface



V_g= -1.0 V

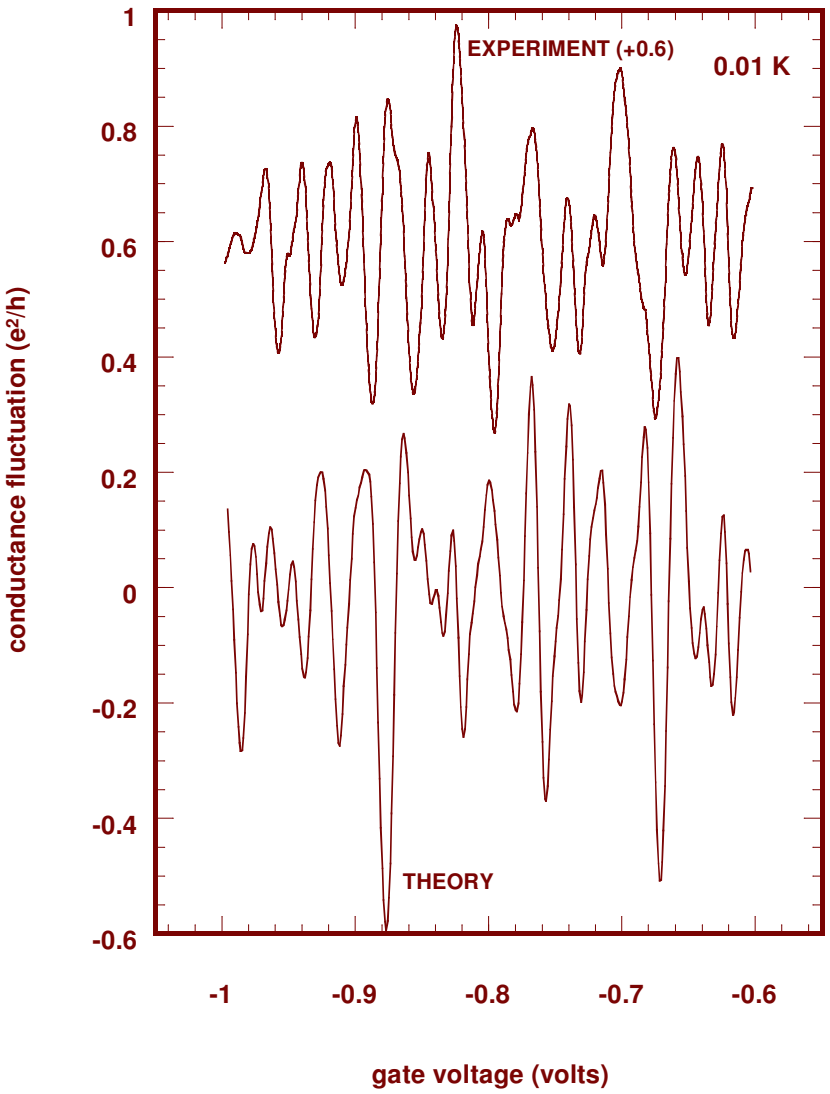


V_g= -0.9 V



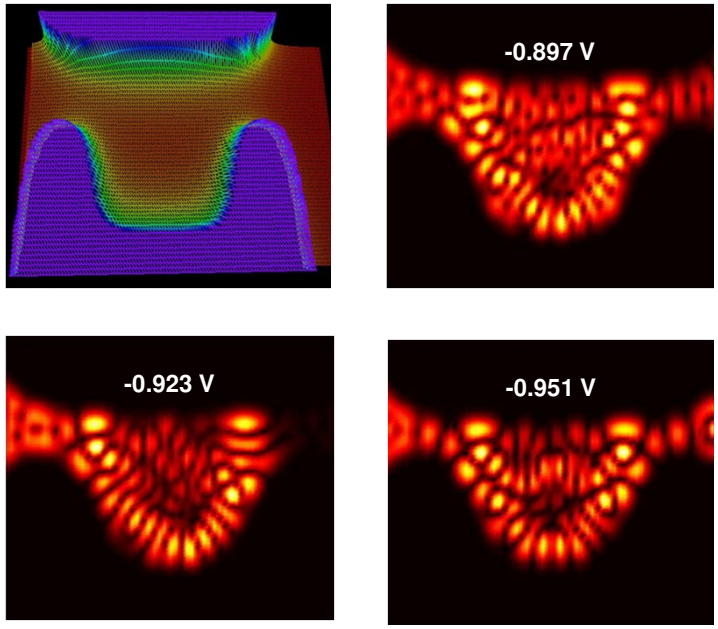
V_g= -0.7 V

Potential evolves smoothly- calculate a few as a function of V_g, and create the rest by interpolation



Subtracting out a background that removes the underlying steps you get periodic fluctuations as a function of gate voltage.

Theory and experiment agree very well



Same simulations also reveal that certain scars may RECUR as gate voltage is varied. The resulting periodicity agrees WELL with that of the conductance oscillations

*** Persistence of the scarring at zero magnetic field indicates its INTRINSIC nature**

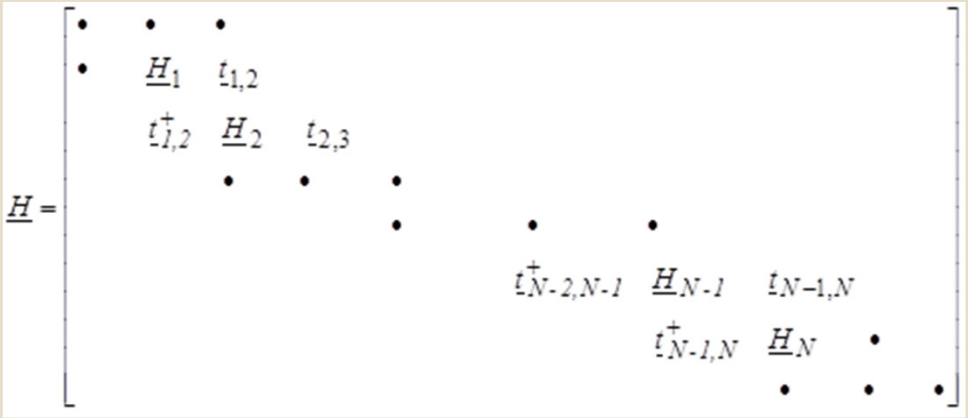
⇒ The scarring is NOT induced by the application of the magnetic field

Quantum Transport

RECURSIVE GREEN'S FUNCTIONS APPROACH

Tight-Binding Hamiltonian

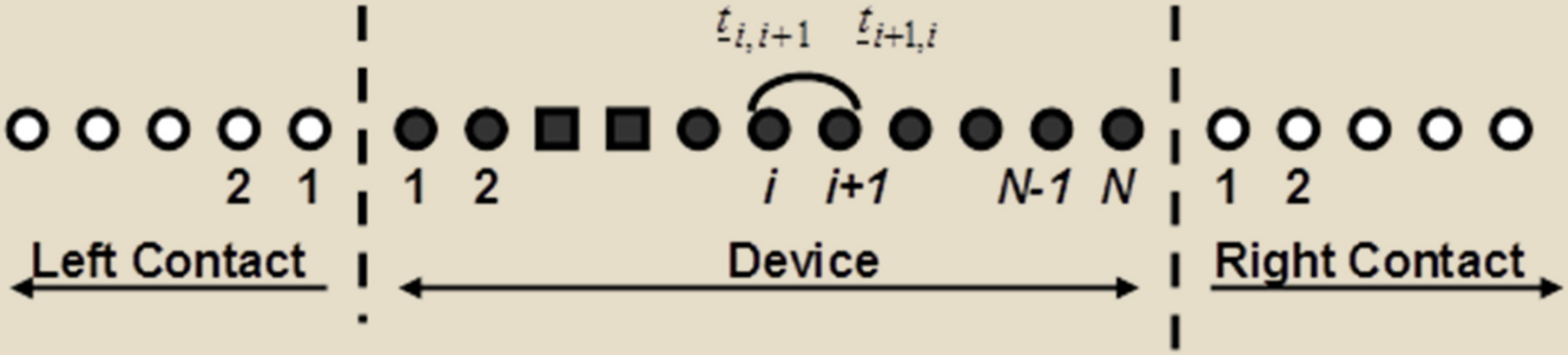
- Divide the whole 1D device structure into points which interact with neighboring points through a coupling constant.
- In the **tight-binding method** one can take the basis functions to be any set of localized functions such as atomic *s*- and *p*-orbitals, Wannier functions, and so forth.
- A common approximation used to describe the Hamiltonian of layered structures consists of non-vanishing interactions only between nearest neighbor layers. That is, each layer *i* interacts only with itself and its nearest neighbor layers *i-1* and *i+1*.
- Then, the single particle Hamiltonian of the layered structure is a block tri-diagonal matrix, where diagonal blocks represent the Hamiltonian of layer *i* and off-diagonal blocks represent interactions between layers *i* and *i+1*:



Matrix Representation of the Kinetic Equations

$$\left[E\underline{I} - \underline{H} - \underline{\Sigma}_B^r - \underline{\Sigma}_{Scat}^r \right] \underline{G}^r = \underline{I}$$

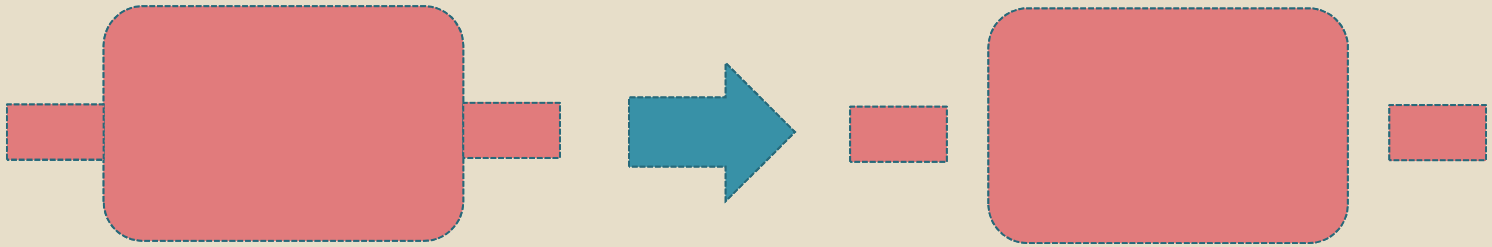
$$\underline{G}^{>,<} = \underline{G}^r \left(\underline{\Sigma}_{\mathrm{B}}^{>,<} + \underline{\Sigma}_{\mathrm{Scat}}^{>,<} \right) \underline{\mathrm{G}}^{\mathrm{a}}$$



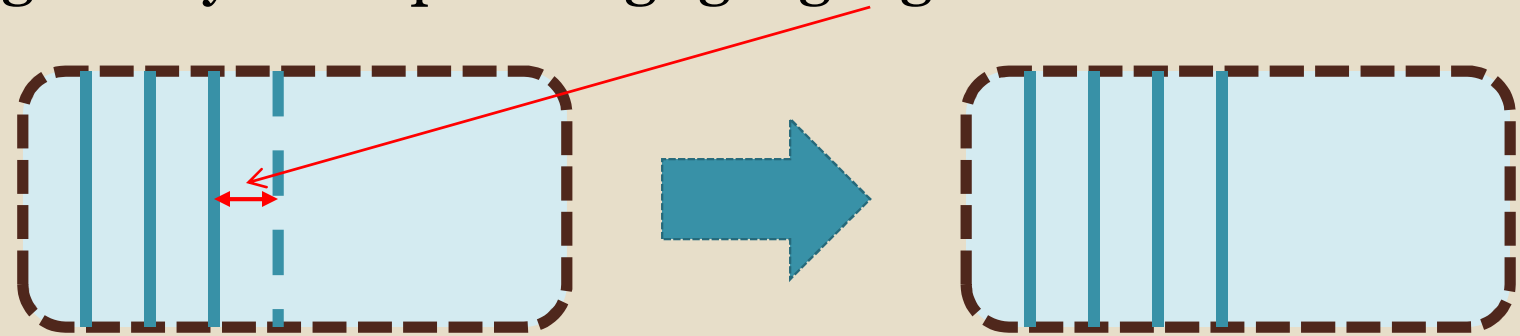
K. B. Kahen, Recursive-Green's-function analysis of wave propagation in two-dimensional nonhomogeneous media, .Phys. Rev. E 47, 2927 - 2933 (1993).

Recursive Green's Function Method at Work

1. Divide the system into leads and internal domain

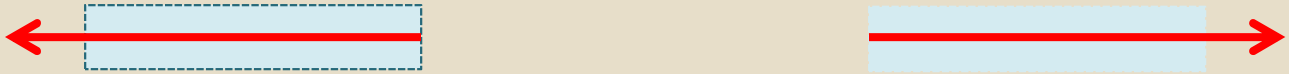


2. Calculate the Green's Function of the internal structure using the Dyson Equation $g=g^0+g^0Vg$

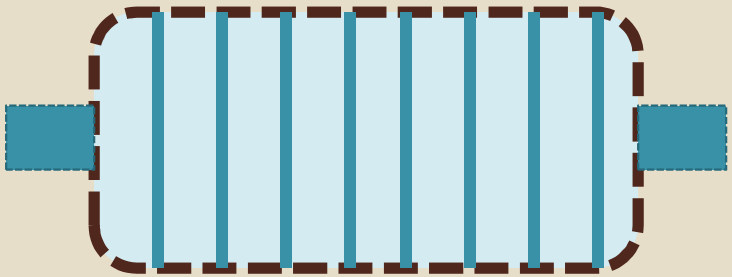


Recursive Green's Function Method at Work

3. Calculate Green's functions of the semi-infinite leads → Surface Green's function (self energy)



4. Use the Dyson Equation to connect the two domains of the system



$$g^{r\,v}_{L_{1,1}} = \frac{A^2_{L_1} + t_1^2 - t_2^{v^2} - \sqrt{\left[A^2_{L_1} + t_1^2 - t_2^{v^2}\right]^2 - 4A^2_{L_1} t_1^2}}{2A^2_{L_1} t_1^2}$$

$$\Sigma^{r\,v}_{L} = t_1^2 g^{r\,v}_{L_{1,1}}$$

Recursive Green's Function Method at Work

Left-connected Green's function:

$$\underline{A}_{1,1}\,\underline{g}^{Lr}_{1,1} = \underline{I}_{1,1} \qquad \underline{A} = \left[E\underline{I} - \underline{H} - \underline{\Sigma}^{r} \right]$$

$$\underline{g}^{Lr}_{q+1,q+1} = \left(\underline{A}_{q+1,q+1} - \underline{A}_{q+1,q}\,\underline{g}^{Lr}_{q,q}\,\underline{A}_{q,q+1} \right)^{-1}$$

Right-connected Green's function:

$$\underline{A}_{N,N}\,\underline{g}^{Rr}_{N,N} = \underline{I}_{N,N}$$

$$\underline{g}^{Rr}_{q-1,q-1} = \left(\underline{A}_{q-1,q-1} - \underline{A}_{q-1,q}\,\underline{g}^{Rr}_{q,q}\,\underline{A}_{q,q-1} \right)^{-1}$$

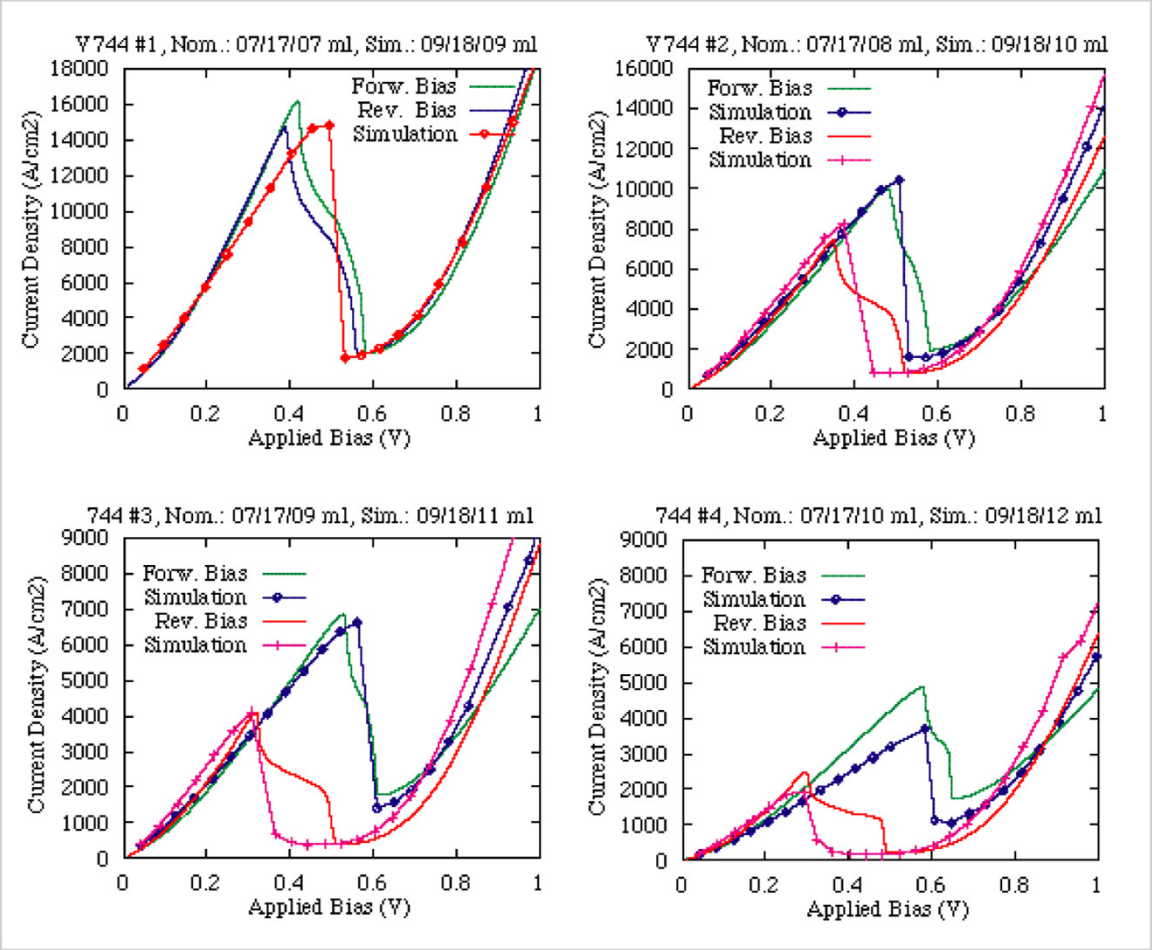
Green's functions needed for transmission coefficient and electron density calculations

$$\underline{G}^{r}_{q,q} = \underline{g}^{Lr}_{q,q} + \underline{g}^{Lr}_{q,q} \left(\underline{A}_{q,q+1}\,\underline{G}^{r}_{q+1,q+1}\,\underline{A}_{q+1,q} \right) \underline{g}^{Lr}_{q,q}$$

$$\underline{G}^{r}_{q+1,q+1} = \underline{g}^{Rr}_{q+1,q+1} + \underline{g}^{Rr}_{q+1,q+1} \left(\underline{A}_{q+1,q}\,\underline{G}^{r}_{q,q}\,\underline{A}_{q,q+1} \right) \underline{g}^{Rr}_{q,q}$$

Example: Simulation of a RTD with NEMO1D

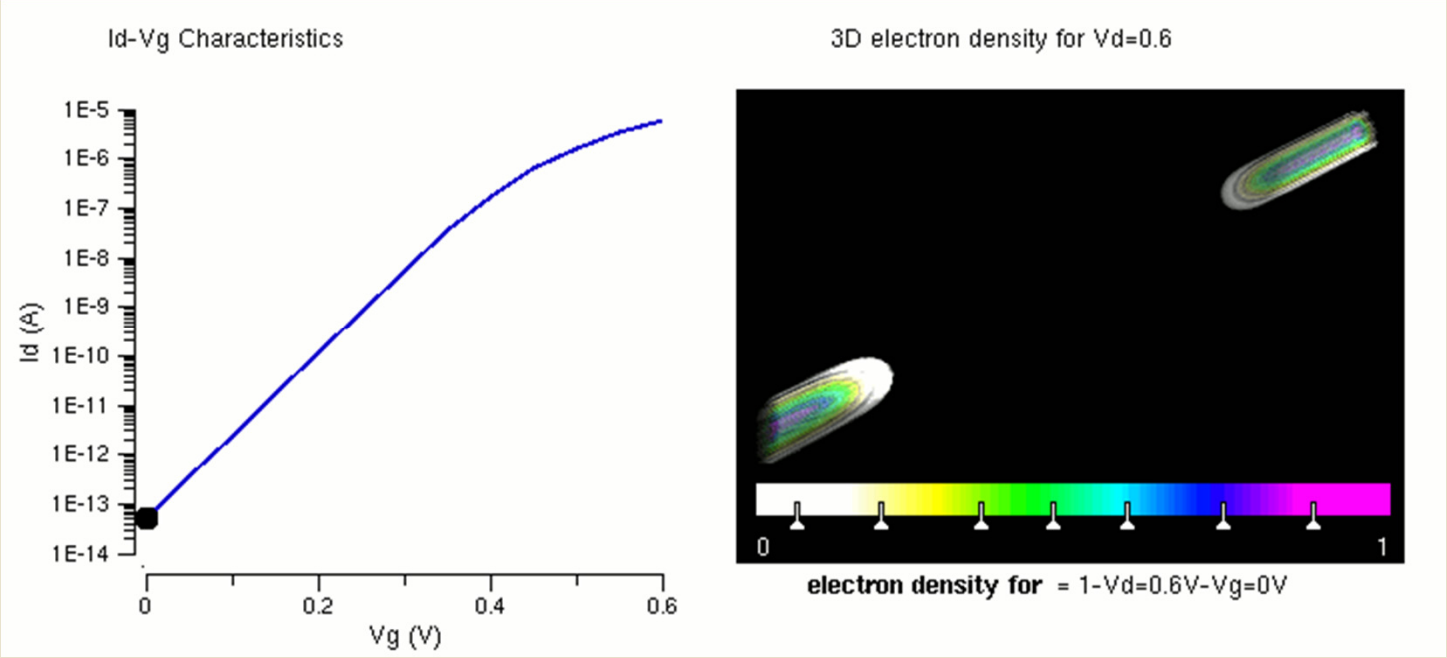
NEMO1D: InGaAs/AlAs RTDs



G. Klimeck, private communication..

Example: Simulation of a Nanowire MOSFET with OMEN

OMEN: Modeling of Nanowire Transistors



Simulation result for formation of inversion channel (electron density) and attainment of threshold voltage (IV) in a nanowire MOSFET. Note that the threshold voltage for this device lies around 0.45V

G. Klimeck, private communication..

Quantum Transport

CONTACT BLOCK REDUCTION METHOD

Direct Solution of the Problem is Time Consuming

The retarded Green's function of an open system:

$$\mathbf{G}^R(E) = [\mathbf{I}E - \mathbf{H}]^{-1} = [\mathbf{I}E - \mathbf{H}^0 - \boldsymbol{\Sigma}]^{-1}$$

where $\mathbf{H}^0$ **⇒ closed system Hamiltonian ,** Σ **⇒ self-energy matrix**

The Dyson equation,

$$\mathbf{G}^R(E) = \left[\mathbf{I} - \mathbf{G}^0(E)\boldsymbol{\Sigma}(E)\right]^{-1}\mathbf{G}^0(E),$$

where

$$\mathbf{G}^0(E) \equiv \left[\mathbf{I}E - \mathbf{H}^0 + i\eta\right]^{-1} = \sum_\alpha \frac{|\alpha\rangle\langle\alpha|}{E - \varepsilon_\alpha + i\eta}\bigg|_{\eta=0^+}, \qquad \mathbf{H}^0|\alpha\rangle = E_\alpha|\alpha$$

$\mathbf{G}^0(E)$ **describes closed system (decoupled device)**

To determine Green's function of an open system we need to invert a huge matrix

D. Mamaluy, D. Vasileska, M. Sabathil, T. Zibold, and P. Vogl, "Contact block reduction method for ballistic transport and carrier densities of open nanostructures", Phys. Rev. B 71, 245321 (2005).

The CBR Algorithm

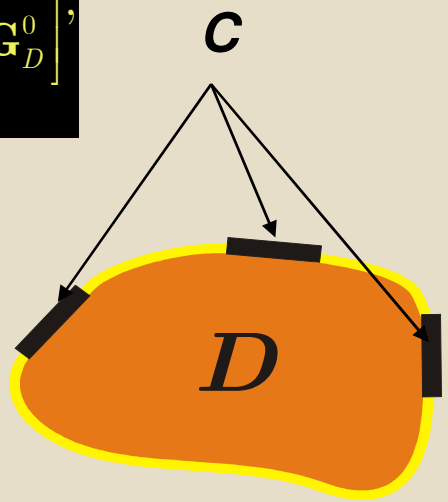
$\mathbf{G}^R$ of an open system in CBR formalism:

$$\mathbf{G}^R = \begin{bmatrix} \mathbf{G}^R_C & \mathbf{G}^R_{CD} \\ \mathbf{G}^R_{DC} & \mathbf{G}^R_D \end{bmatrix} = \begin{bmatrix} \mathbf{A}_C^{-1}\mathbf{G}^0_C & \mathbf{A}_C^{-1}\mathbf{G}^0_{CD} \\ -\mathbf{A}_{DC}\mathbf{A}_C^{-1}\mathbf{G}^0_C + \mathbf{G}^0_{DC} & -\mathbf{A}_{DC}\mathbf{A}_C^{-1}\mathbf{G}^0_{CD} + \mathbf{G}^0_D \end{bmatrix},$$

$$\mathbf{A}_C = 1_C - \mathbf{G}^0_C\Sigma_C, \mathbf{A}_{DC} = -\mathbf{G}^0_{DC}\Sigma_C$$

$\mathbf{G}^0_C$ is the contact portion of the $\mathbf{G}^0$

where,
index *D* denotes the interior device region
index *C* denotes the contact (boundary) region



All elements of G^R can be determined from inversion of small matrix A_C

- The left upper block $\mathbf{G}^R_C$ fully determine the transmission function
- The left lower block $\mathbf{G}^R_{DC}$ determines density of states, charge density etc.

Transmission Coefficient and Electron Density

- Transmission Function

$$T_{\lambda\lambda'}(E) = Tr(\mathbf{\Gamma}^{\lambda} \boldsymbol{G}^{R} \mathbf{\Gamma}^{\lambda'} \boldsymbol{G}^{R\dagger})$$

  - CBR Formalism

$$T_{\lambda\lambda'}(E) = Tr(\mathbf{\Gamma}_C^{\lambda} \boldsymbol{G}_C^{R} \mathbf{\Gamma}_C^{\lambda'} \boldsymbol{G}_C^{R\dagger}), \text{ where } \boldsymbol{G}_C^{R} = [\mathbf{1} - \boldsymbol{G}_C^{0} \mathbf{\Sigma}_C]^{-1} \boldsymbol{G}_C^{0} \quad \mathbf{\Gamma}_C^{\lambda} = i[\mathbf{\Sigma}_C - \mathbf{\Sigma}_C^{\dagger}]$$

- Local Density of States Function

$$\rho(\mathbf{r}, E) = \left\langle \mathbf{r} \mid \mathbf{G}^{R} \mathbf{\Gamma} \mathbf{G}^{R\dagger} \mid \mathbf{r} \right\rangle / 2\pi$$

  - CBR Formalism

$$\rho(\mathbf{r}, E) = \frac{1}{2\pi} \sum_{m} \left| \boldsymbol{G}_{\mathbf{r}m}^{R} \right|^2 \mathbf{\Gamma}_{mm},$$

$$\boldsymbol{G}_{\mathbf{r}m}^{R} = \left\langle \mathbf{r} \mid \mathbf{G}_{DC}^{0} \mathbf{B}_C^{-1} \mid m \right\rangle = \sum_{m',\alpha} \frac{\left\langle \mathbf{r} \mid \alpha \right\rangle \left\langle \alpha \mid m' \right\rangle}{E - \varepsilon_{\alpha} + i\eta} \Bigg|_{\eta=0^{+}} \left\langle m' \mid \mathbf{B}_C^{-1} \mid m \right\rangle$$

Complexity of CBR vs. Other Algorithms

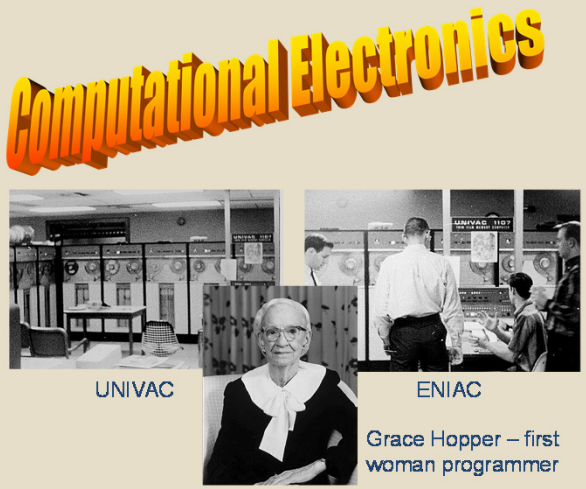
Method	Computational cost
Transfer matrix + QTBM	$N_E \times O\left(N_{TOTAL}^3\right)$
NanoMOS (Purdue University)	$N_E \times N_x \times O\left(\left[N_y N_z\right]^2\right) \approx N_E \times O\left(N_{TOTAL}^{5/3}\right)$
QDAME (IBM, S. Laux)	$N_{TOTAL} \times O\left(N_{eigen}^2\right) + N_E \times O\left(N_{TOTAL}^{3/2}\right)$
CBR	$N_{TOTAL} \times O\left(N_{eigen}^2\right) + N_E \times O\left(N_{TOTAL}\right)$
Notations N_E : number of energy steps; N_{TOTAL} : number of grid points N_{eigen} : number of eigenvalues	**CBR WINS !!!**

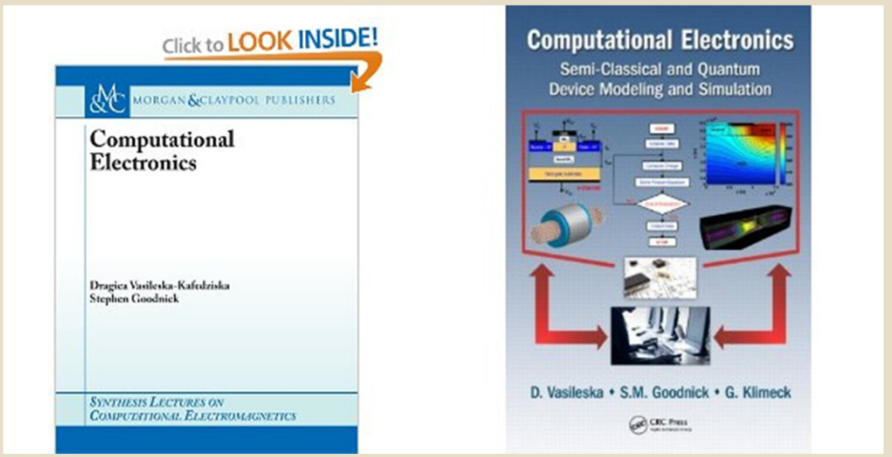
What are the Proper Transport Models at the Nanoscale?

Semiclassical Transport Approaches

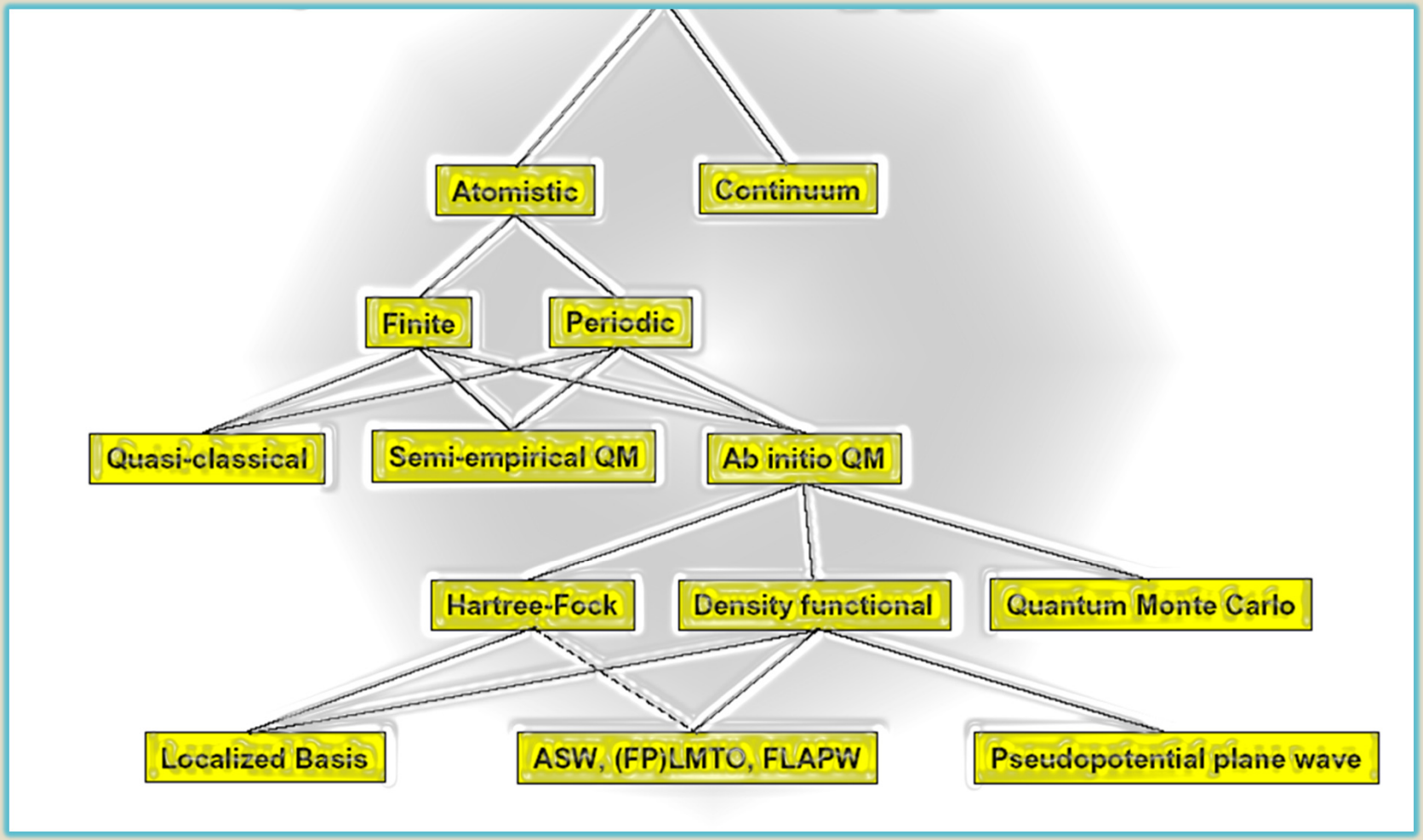
Quantum Transport

Atomistic Simulations





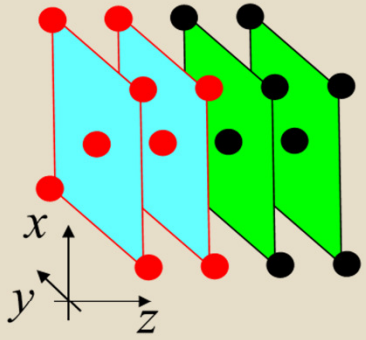
First Principles Calculations



Self-Consistent Tight Binding Calculations

[A. Di Carlo et. al., Solid State Comm. 98, 803 (1996); APL 74, 2002 (1999)]

The electron and hole densities in each 2D layer are given by:



$$n(z) = \frac{1}{(2\pi)^2} \int_{BZ_{//}} d^2\mathbf{k}_{//} \sum_c \left| \langle z | E_c \mathbf{k}_{//} \rangle \right|^2 f(E_c - F_n)$$

$$p(z) = \frac{1}{(2\pi)^2} \int_{BZ_{//}} d^2\mathbf{k}_{//} \sum_v \left| \langle z | E_v \mathbf{k}_{//} \rangle \right|^2 (1 - f(F_h - E_v))$$

The influence of free carrier charge redistribution and macroscopic polarization fields are included by solving the *Poisson equation:*

$$\frac{d}{dz} D(z) = \frac{d}{dz}\left(-\varepsilon \frac{d}{dz} V_H + P \right) = e\left(p - n + N_D^+ - N_A^-\right)$$

+ boundary conditions

$$H = H_C + V_H \Rightarrow \left| E_i \mathbf{k}_{//} \right\rangle$$

A. Di Carlo, Private Communication.

Boundary Conditions for Transport

The transport problem is:

active region where symmetry is lost
+
contact regions (semi-infinite bulk)

Open-boundary conditions can be treated within several schemes:

- Transfer matrix
- Green Functions

These schemes are well suited for localized orbital approach like TB

A. Di Carlo, Private Communication.

Conclusions

- Nanoelectronics has revolutionized in many ways our every day life.
- It has made significant impact in fields like medicine in terms of diagnostics and surgical interventions.
- There are many alternative paths and ways in which future nanoelectronics research might go.
- Atomistic simulations will definitely be of crucial importance and need for understanding future nanoelectronic devices
- Parallel computing will be essential for performing multi-million atomistic simulations.