Nanoelectronic Modeling (NEMO)  
Motivation and Background  

Gerhard Klimeck  
Dragica Vasileska
1965 Gordon Moore => Moore’s Law

http://www.intel.com/technology/mooreslaw

Relative Manufacturing Cost per Component

Number of Components per Integrated Circuit
Moore’s Law
a Self-Fulfilling Prophesy

• From

Gerhard Klimeck
Technical Developments to enable Moore’s Law

Robert Chau (Intel), 2004
Today’s CPU Architecture

Heat becoming an unmanageable problem
1. Increased costs for R&D and production facilities, which are becoming too large for any one company or country to accept.
2. Shorter process technology life cycles.
3. Emphasis on faster characterization of manufacturing processes, assisted by modeling and simulation.
TCAD: Technology for Computer Aided Design

- Evaluating "what-if" scenarios rapidly
- Providing problem diagnostics
- Providing full-field, in-depth understanding
- Providing insight into extremely complex problems/phenomena/product sets
- Decreasing design cycle time (savings on hardware build lead-time, gain insight for next product/process)

1. Shortening time to market
Some TCAD Prerequisites Are:

• Modeling and simulation require enormous technical depth and expertise not only in simulation techniques and tools but also in the fields of physics and chemistry.

• Laboratory infrastructure and experimental expertise are essential for both model verification and input parameter evaluations in order to have truly effective and predictive simulations.

• Software and tool vendors need to be closely tied to development activities in the research and development laboratories.

R. Dutton, Stanford University, the father of TCAD.
1964: Gummel introduced the decoupled scheme for the solution of the Poisson and the continuity equations for a BJT

1968: de Mari introduced the scaling of variables that is used even today and prevents effectively overflows and underflows

1969: Sharfetter and Gummel, in their seminal paper that describes the simulation of a 1D Silicon Read (IMPATT) diode, introduced the so-called Sharfetter-Gummel discretization of the continuity equation

Coupling of Transport Equations to Poisson and Band-Structure Solvers

D. Vasileska and S.M. Goodnick,
What Transport Models exist?

- Semiclassical **FLUID** models (ATLAS, Sentaurus, Padre)
  - Drift – Diffusion
  - Hydrodynamics

1. Particle density
2. DRIFT VELOCITY, ENERGY DENSITY
3. velocity overshoot effect

**Problems**

**Graphs:**
- **Drift velocity vs. Electric field**
  - Current simulations
  - Yamada simulations
  - Canali exp. data

**Drain Voltage vs. Drain Current**
- **S-Places2B**
• Semi-classical PARTICLE-BASED Models:
  » Direct solution of the BTE Using Monte Carlo method

  ✓ Eliminates the problem of Energy Relaxation Time Choice
  ✓ Accurate up to semi-classical limits
  ✓ One can describe scattering very well
  ✓ Can treat ballistic transport in devices
1. Quantum Mechanical TUNNELING

2. SIZE-QUANTIZATION

3. QUANTUM INTERFERENCE EFFECT
What Quantum Transport Models Exist?

• Quantum-mechanical **WIGNER** Function and **DENSITY** Matrix Methods:
  » Can deal with correlations in space
  » BUT NOT WITH CORRELATIONS IN TIME

**Advantages:** Can treat SCATTERING
**Disadvantages:** LONG SIMULATION TIMES
Non-Equilibrium Green’s Functions (NEGF)

- MOST fundamental and accurate
- Considered by many to be the MOST difficult quantum approach
- FORMULATION OF SCATTERING rather straightforward and theoretically sound including incoherence and irreversibility
- IMPLEMENTATION OF SCATTERING rather difficult
- Computationally INTENSIVE
# Length Scales and Interactions

Determine the Most Appropriate Model

<table>
<thead>
<tr>
<th>Transport Regime</th>
<th>( L &lt;&lt; l_{e-ph} )</th>
<th>( L \sim l_{e-ph} )</th>
<th>( L &gt;&gt; l_{e-ph} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( L &lt; \lambda )</td>
<td>Quantum \hspace{1cm} Ballistic \hspace{1cm} Fluid \hspace{1cm} Fluid</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( L &lt; l_{e-e} )</td>
<td>Rare \hspace{1cm} Rare \hspace{1cm} ( e-e ) (Many), ( e-ph ) (Few) \hspace{1cm} Many</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( L &gt;&gt; l_{e-e} )</td>
<td>\hspace{1cm} \hspace{1cm} \hspace{1cm} \hspace{1cm}</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Model:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drift-Diffusion</td>
</tr>
<tr>
<td>\hspace{1cm} Quantum Hydrodynamic</td>
</tr>
<tr>
<td>Hydrodynamic</td>
</tr>
<tr>
<td>\hspace{1cm}</td>
</tr>
<tr>
<td>Monte Carlo</td>
</tr>
<tr>
<td>\hspace{1cm}</td>
</tr>
<tr>
<td>Schrodinger/Green’s Functions</td>
</tr>
<tr>
<td>Wave</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Applications</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nanowires, Superlattices</td>
</tr>
<tr>
<td>Ballistic</td>
</tr>
<tr>
<td>Transistor</td>
</tr>
<tr>
<td>Current IC’s</td>
</tr>
<tr>
<td>Current IC’s</td>
</tr>
<tr>
<td>Older IC’s</td>
</tr>
</tbody>
</table>
Robert Chau (Intel), 2004

- Industry plans have a 5-10 year horizon
- Industry has been on time:
  - 32nm node predicted in 2004 and announced 2009
- There are NO technically viable solutions beyond 2015
**Exponential performance increase:**
- Enabled by:
  - **device miniaturization**
  - chip size increase
- Limited by:
  - Costs of fabrication

---

**Moore’s Law for Lithography**

- SIA projection for SRAM

---

**2D Feature**

- 1-D feature
- 5-100 Å

---

**Growth**
A Third Look at Moore’s Law
Countable number of electrons

Exponential performance increase:
- Enabled by
  - **device miniaturization**
  - chip size increase
- Limited by:
  - Costs of fabrication
  - **Discrete atoms/electrons**
Exponential performance increase:
- Enabled by
  - device miniaturization
  - chip size increase
- Limited by:
  - Costs of fabrication
  - Discrete atoms/electrons

Quantum Dots
- Artificial Atoms - Electron Boxes

1D Heterostructures
- Lasers and detectors
- Fast electronic devices
**Device Trends and Challenges**

**Questions / Challenges**
- Strain?
- Quantization?
- Crystal orientation?
- Atoms are countable; does granularity matter? Disorder?
- New material or new device?

**Assertions of importance**
- High bias / non-equilibrium
- Quantum mechanics
- Atomistic representation
  - Band coupling, non-parabolicity, valley splitting
  - Local (dis)order, strain and orientation

**Observations:**
- 3D spatial variations on nm scale
- Potential variations on nm scale
- New channel materials (Ge, III-V)
Quantum Transport far from Equilibrium

**Macroscopic dimensions**

**Non-Equilibrium Quantum Statistical Mechanics**

**Drift / Diffusion**

**Unified model**

**Boltzmann Transport**

**Quantum**

**Diffusive**

**Ballistic**

**Non-Equilibrium Green Functions**

Macroscopic dimensions:

\[ \rho = \exp\left(-\frac{H - \mu N}{kT}\right) \]

\[ \mu_{1}, \mu_{2} \]

\[ \Sigma_{1}, \Sigma_{2} \]

\[ \sum_{s} \]

SILICON

INSULATOR

\[ V_{G}, V_{D} \]

\[ -I \rightarrow \]

\[ \mu_{1} \]

\[ \mu_{2} \]
The non-equilibrium Green function formalism underlies NEMO.
All of the approaches shown were considered.
Approaches in light blue were dropped. Approaches in dark blue were incorporated.
Semiconductor Industry has Fundamental Issues and Problems

- Driven by a revenue stream –
  => it must be cheaper and better
  => so people throw away their old computers

- Devices are at the nanometer scale
  => wavelength of the electrons
  !!! Existing tools are not fundamentally quantum mechanics based

- Devices now consist of “countable number of atoms
  => does the atomistic granularity matter?
  !!! Existing tools are based on continuum matter theory

- Devices consume too much heat
  => are there alternative designs?
  !!! Existing tools cannot handle QM, atomistic granularity, and thermal transport
• Production level, industrial semiconductor devices:
  » Show spatial arrangements in 3D – no longer planar
  » Have dimensions where atoms are countable
  » Involve new materials
• Fundamental theory for modeling
  » Needs to include high bias and carrier interactions
  » Needs to be on an atomistic basis
  » Has been developed: NEGF-Non-Equilibrium Green Functions
• Model implementations:
  » Must be validated against experimental data
  » Predictive
  » Deliver physical insight
  » Computationally efficient
• Must be taught to the next generation engineers!