Parallel Ensemble Monte Carlo for Device Simulation

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Outline

- Electronic transport problems and solutions
  - Semiclassical transport theory
  - Boltzmann transport equation and its solutions
  - Simulation vs Monte Carlo
  - The Monte Carlo procedure
- Parallel ensemble Monte Carlo algorithm
  - Inherently parallel and synchronous
- Why and When Use Monte Carlo
  - Validity of Assumptions
  - Incentive for using Monte Carlo
- Applications
Spectrum of Approaches to Electronic Transport and Systems

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Parallel Ensemble Monte Carlo for Device Simulation

The “Big Picture”

Physics

Device

Quantum mechanical

Monte Carlo

Semiclassical

Relaxation-time approx

Drift-diffusion

Circuit

Device

Circuit

Logic

Electrical

Behavioral

Timing

Switch

Gate

RTL

Engineering

System

Functional

Structural

Behavioral

DD

MC

Timing

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Electrical

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Quantum mechanical

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Physics

Engineering

The “Big Picture”
Central assumption — a single carrier distribution function, \( f(r,k,t) \), exists which may be used to compute statistical expectation values for macroscopic current flows.

Corner-stone — the Boltzmann transport equation (BTE)

- Equation of motion for \( f(r,k,t) \), the probability of finding a particle with crystal momentum \( \hbar k \) at position \( r \) and time \( t \)

\[
\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_r f - q \mathbf{E} \cdot \nabla_p f = \int dp' \left[ f(p') S(p',p) - f(p) S(p,p') \right]
\]

Macroscopic quantity

\[
\langle A(r,t) \rangle = C \int A(r,k,t) f(r,k,t) \, d^3k
\]

e.g., \( J(r,t) = \frac{q}{4\pi^3} \int v(k) f(r,k,t) \, d^3k \)
Solutions to the Boltzmann Transport Equation

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BTE

- inverse
- Path integral
  - numerical
  - Iterative
  - Monte Carlo
- 2nd moment
  - Balance equation
    - $f(T_e, V_d)$
    - $\tau_m, \tau_E$
  - Drift-diffusion
    - Current continuity Poisson
    - $\mu, D$
    - $\mu(F), D(F)$
    - Hot-electron effects
- 1st moment
- Semiempirical transport eq.
  - Displaced Maxwellian
  - Semiconductor equations
Simulation vs Monte Carlo Approach

Nonlinear integro-differential equation

Approximation
Partial differential equations
Finite difference
Finite element
Numerical simulation

Physical model

Transformation
Numerical model
Path integral

Discretization

Solution

Particle model
Monte Carlo
Example — **Calculation of π**: Collect rain drops in both the circle and its circumscribed square, and find the fraction that lies in the circle

\[ I = \int_0^1 \int_0^{\sqrt{1-x^2}} dx dy = \frac{\pi}{4} = 0.785398 \ldots \]

**Simulation Approach**

\[ I = \int_0^1 \sqrt{1-x^2} dx \approx I_n = \frac{1}{n} \sum_{i=1}^{n} \sqrt{1-(i/n)^2} \]

**Monte Carlo Approach**

Generate random pairs \((x_r, y_r)\) using uniformly distributed random numbers \(r \in [0,1]\), and count the fraction that lies inside the circle: \(|r - r_0| \leq 1\)
Monte Carlo Approach to Device Simulation

Procedure

- **Path traversal**: governed by classical laws of motion and terminated at a time $t_f$ selected on a random value of the function $\exp(-Gt)$ (“time of free flight”)

  $$t_f = -\ln r/G$$

- **Scattering**: from the state at the end of this traverse to a new state according to the microscopic probability of the scattering process, also determined using random numbers

Estimator

- The distribution of the states $(k_i, E_i)$ on a $k$-space grid becomes a representation of $f(k)$. An estimator is obtained from:

  $$\langle A \rangle = \sum_{i=1}^{N_f} \frac{A(k_i)}{N_f}$$
Visualizing the Monte Carlo Process

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**Parallel Ensemble Monte Carlo for Device Simulation**

\[ t = 0 \quad \text{transient} \quad t = n\Delta t \quad \text{steady state} \]

\[ \text{B.C.}(0) \quad \text{S}(0) = S_0 \]

\[ \text{B.C.}(t) \quad \text{S}(t) \]

Computational box

**Free-flight — scattering — sampling**

- real scattering
- self-scattering

**Synchronous-ensemble method**

- scattering events

Distance

\[ z \]

Time

\[ t^{(n-1)} \quad t^{(n)} \]

\[ t_1 \quad t_2 \quad t_i \quad t_N \]

\[ t_f \]

\[ t \]

\[ \Delta t \]
Sequential vs Parallel Monte Carlo Flowchart

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Preliminary calculation
Initial condition of motion

Charge assignment
Poisson solver

n = 1 to N

Single-particle Monte Carlo

Ensemble average
\[ A = \frac{1}{N} \sum_{i=1}^{N} A_i \]

\[ t = t + \Delta t \]

No

Yes

Stop

Parallel Ensemble Monte Carlo

n = 1 to M

Single-particle Monte Carlo

Sub-ensemble average
\[ A^1 = \frac{1}{M} \sum_{i=1}^{M} A_i \]

k = N/M

\[ A^k = \frac{1}{M} \sum_{i=1}^{M} A_i \]

Ensemble average
\[ A = \frac{1}{N/M} \sum_{k=1}^{N/M} A^k \]
Validity of Assumptions

- **Drift-diffusion formalism** — depends on the 1st moment of the BTE (e.g., $\mu$, $D$)
  - Quasi-thermal equilibrium: $T_e \approx T_L$
  - Local-field approximation: $v(r) = \mu \mathcal{E}(r)$

- **Relaxation-time approximation** — depends on the 2nd moment of the BTE (e.g., $\langle v \rangle$, $\langle E \rangle$)
  - Any perturbation of the distribution function, $f$, from the local equilibrium distribution, $f_0$, will relax back to $f_0$ within a “relaxation time” $\tau_R$
  - Valid when scattering is dominated by either isotropic or elastic mechanisms

- **Semiclassical transport theory (BTE)**
  - “Instantaneous” collision: $\tau_c \ll \tau$
  - “Frequent” scattering: $\tau \ll \tau_d, L > \Lambda$
- nonlocality of scattering
- strong field
- strong scattering
- dense systems
- small systems

- submicron devices
- spatial/temporal nonlocal effects
- high-field transport
- ultrafast phenomena
- 2D quantization
- memory effects

- submicron devices
- transients
- moderate field
- high carrier density

- long device
- steady state
- low field
- limited hot carrier effect

- long device
- equilibrium
- low field
- low carrier density

Approach — Generate a solution as efficient as possible while retaining the desired level of accuracy
Incentive for Using Parallel Ensemble Monte Carlo

From the physics point of view

- Study of submicron/deep-submicron devices requires new device physics, in addition to new technology and market demand, since most assumptions made in conventional approaches (DD) will no longer be valid
- The gap between present MC models and formulations of quantum transport beyond the BTE is very wide for nearly all devices of current technological importance

From the algorithm point of view

- The Monte Carlo algorithm is simple, the only drawback is CPU intensive
- Ensemble Monte Carlo is inherently parallel and synchronous

From the applications point of view

- When modeling of deep-submicron devices is routinely needed, with the power of high performance parallel supercomputing facilities, the Monte Carlo approach to device simulation will be of commercial value, not just a research tool
Applications

- **Deep-submicron device simulation**
  - Coupled with Poisson equation: MOSFET’s, BJT’s, …
  - Coupled with Schrödinger and Poisson equations: HEMT’s, HBT’s, QW’s, resonant tunneling devices, …

- **Ultrafast science**
  - Coupled with Maxwell’s equation: photocarrier excitation and relaxation, photodetectors, photoconductive switches, electro-optic sampling, …

- **Bulk material and transport study**
  - Novel material properties, new device physics and phenomena, …
  - Extraction of transport parameters \((\mu, D, \tau_m, \tau_E)\) for conventional device simulation
Conclusion

Two driving forces for using Monte Carlo
- Continued decrease in device dimensions
  - Assumptions made in conventional techniques are no longer valid
- Continued increase in CPU speed
  - high performance parallel computing

Two characteristics of Monte Carlo
- Exact solution to the BTE without any \textit{a priori} assumption on the distribution function
- Inherently parallel algorithm

Conclusion: \textit{It won’t be too long before the Monte Carlo approach to device simulation steps out of R&D labs and becomes a routine simulation tool}