Workshop on High Performance Computing Activities in Singapore

Parallel Ensemble Monte Carlo for Device Simulation

Dr Zhou Xing

School of Electrical and Electronic Engineering

Nanyang Technological University

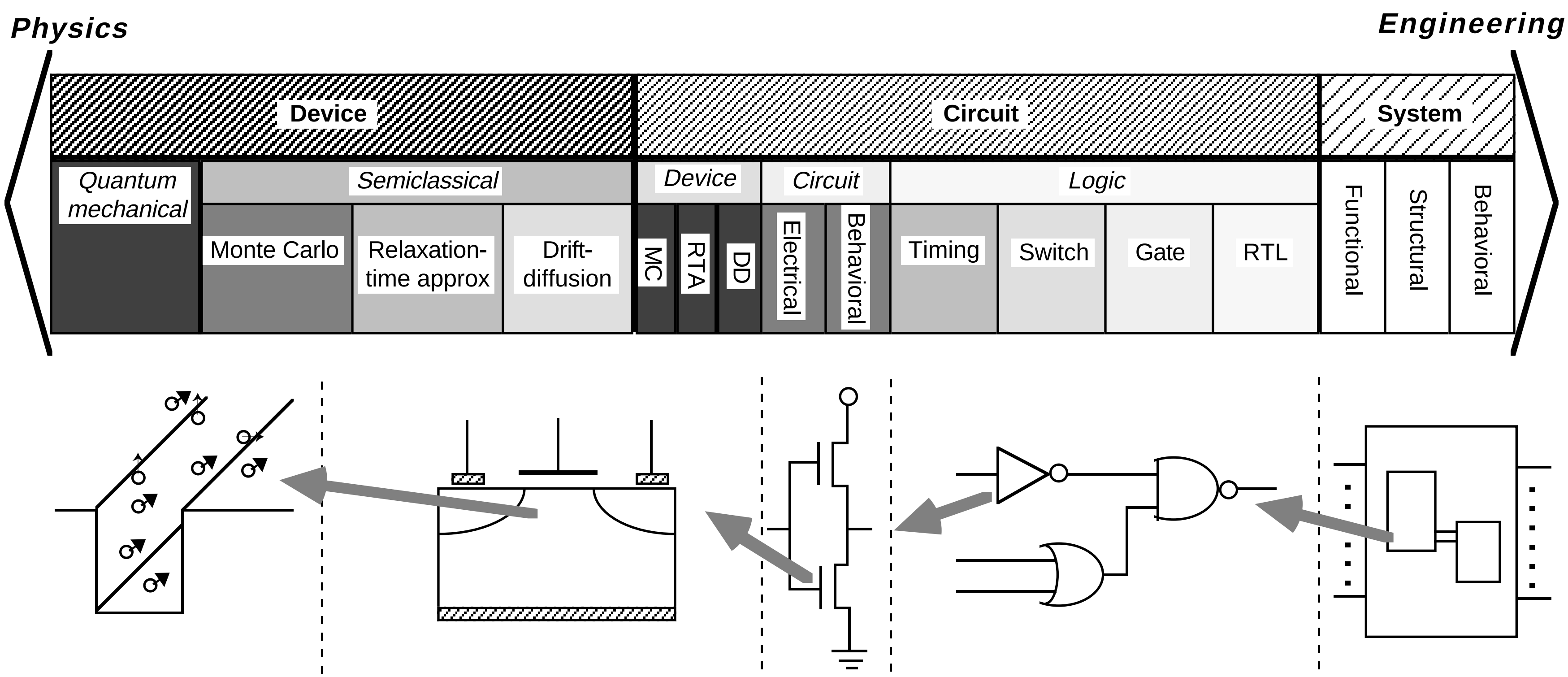
September 29, 1995

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 syncronous
- **Why and When Use Monte Carlo**
  - Validity of Assumptions
  - Incentive for using Monte Carlo
- **Applications**

Spectrum of Approaches to Electronic Transport and Systems

The "Big Picture"



Semiclassical Transport Theory

- **Central assumption** — a single carrier distribution function, $f(\mathbf{r},\mathbf{k},t)$, 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 $f(\mathbf{r},\mathbf{k},t)$, the probability of finding a particle with crystal momentum $\hbar\mathbf{k}$ at position $\mathbf{r}$ and time t

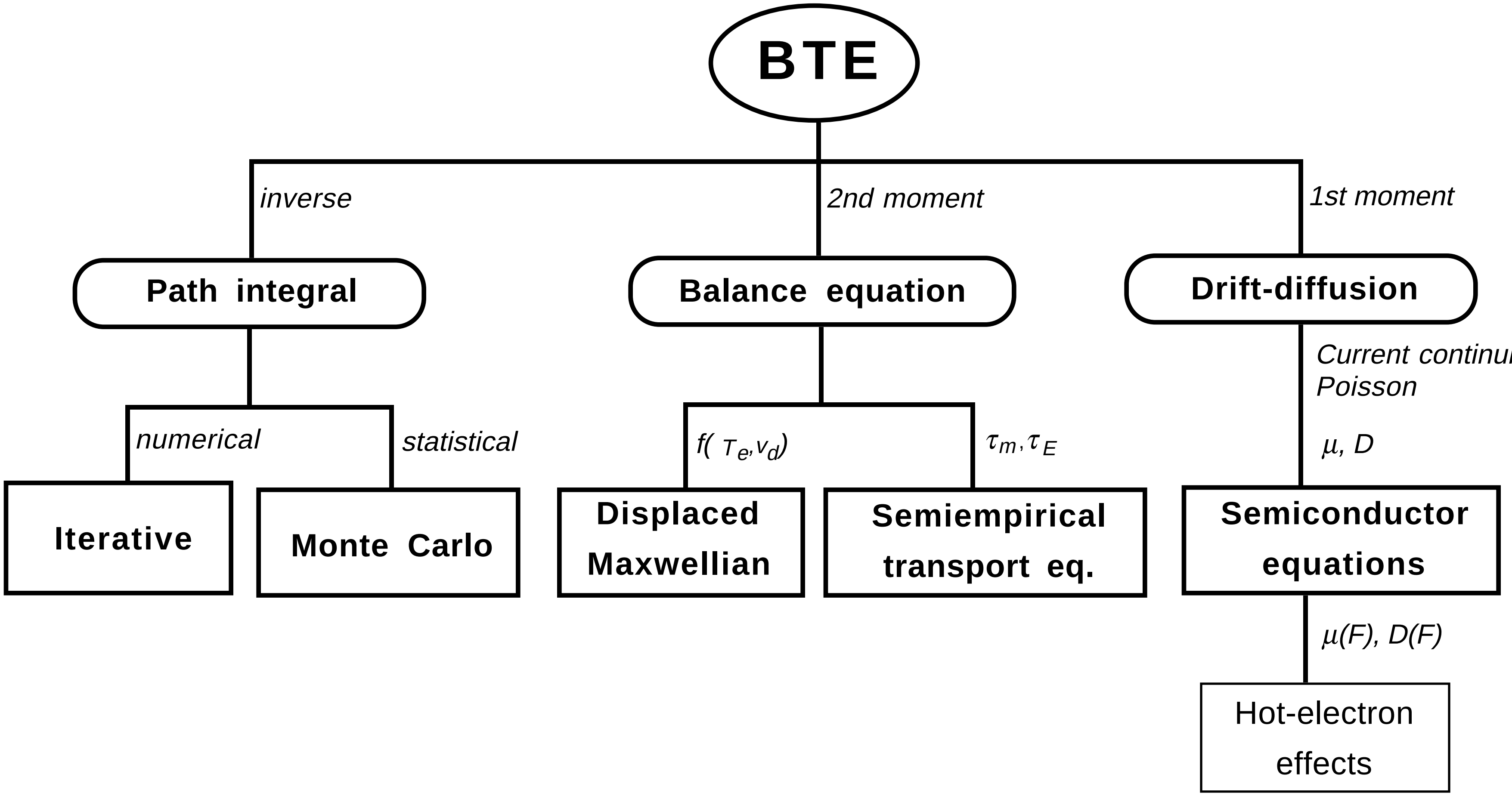
$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f - q\mathcal{E} \cdot \nabla_{\mathbf{p}} f = \int d\mathbf{p}' \left[f(\mathbf{p}') S(\mathbf{p}',\mathbf{p}) - f(\mathbf{p}) S(\mathbf{p},\mathbf{p}') \right]$$

- **Macroscopic quantity**

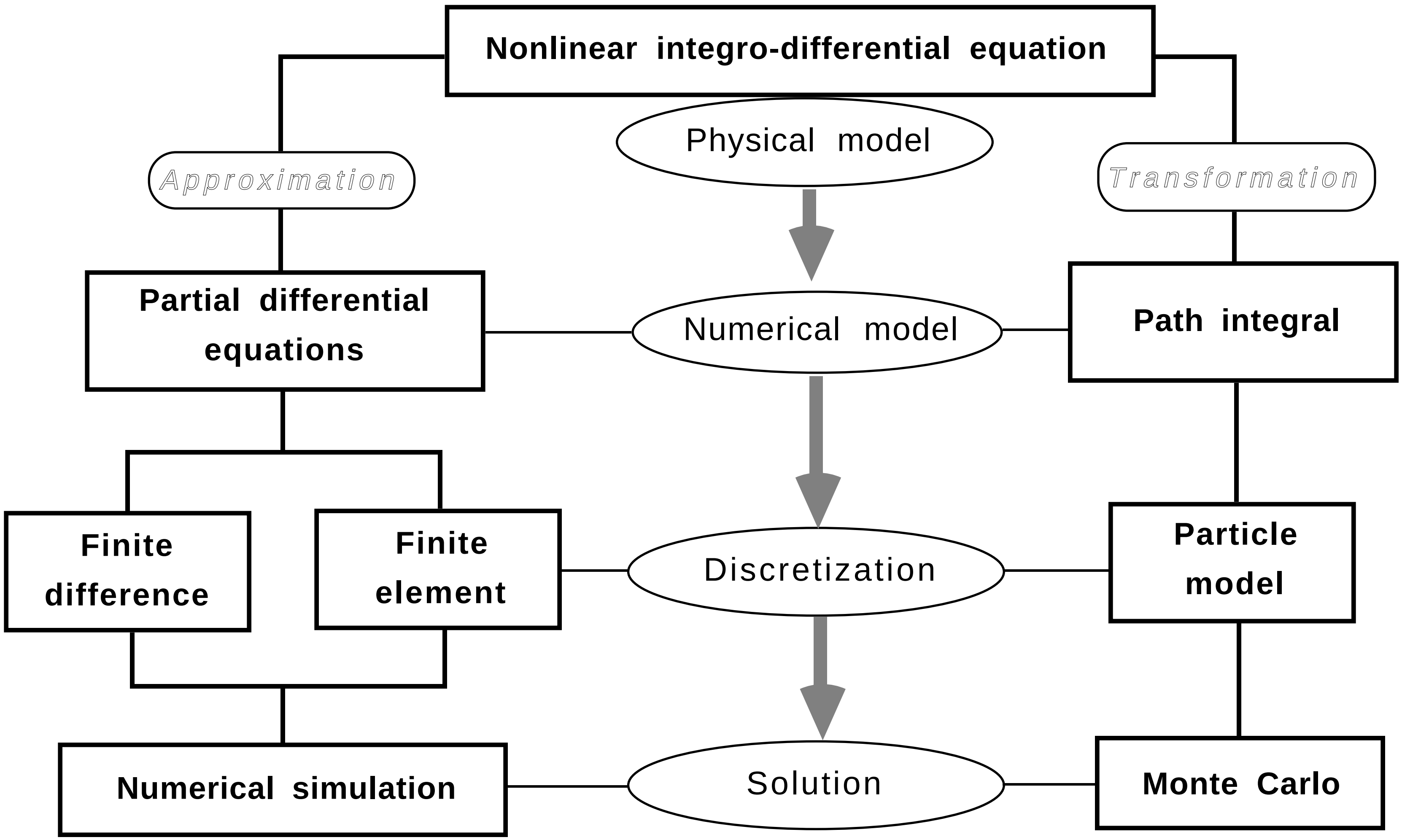
$$\langle A(\mathbf{r},t) \rangle = C \int A(\mathbf{r},\mathbf{k},t)\; f(\mathbf{r},\mathbf{k},t)\; d^3\mathbf{k}$$

$$\text{e.g., } J(\mathbf{r},t) = \frac{q}{4\pi^3} \int v(\mathbf{k})\; f(\mathbf{r},\mathbf{k},t)\; d^3\mathbf{k}$$

Solutions to the Boltzmann Transport Equation

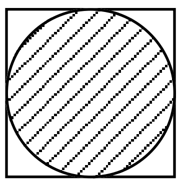


Simulation vs Monte Carlo Approach



Simulation vs Monte Carlo: An Example

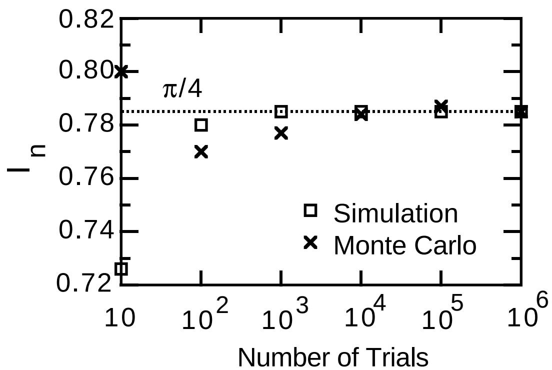
- **Example — *Calculation of* π:** Collect rain drops in both the circle and its circumscribed square, and find the fraction that lies in the circle



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

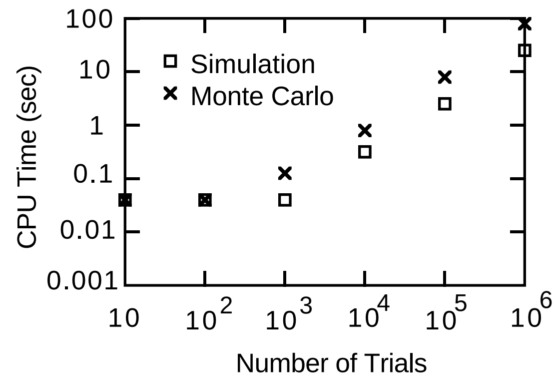
Simulation Approach

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



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: $|\mathbf{r} - \mathbf{r}_0| \leq 1$



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 $\exp(-\Gamma t)$ ("time of free flight")

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

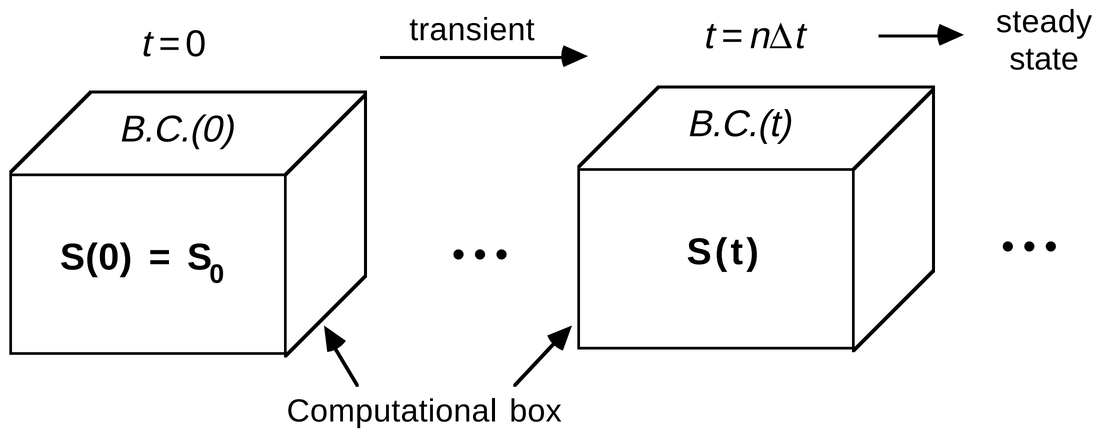
- *Scattering*: from the state at the end of this traverse to a new state according to the microscopic probability of the scattering process, also determined using random numbers

❑ Estimator

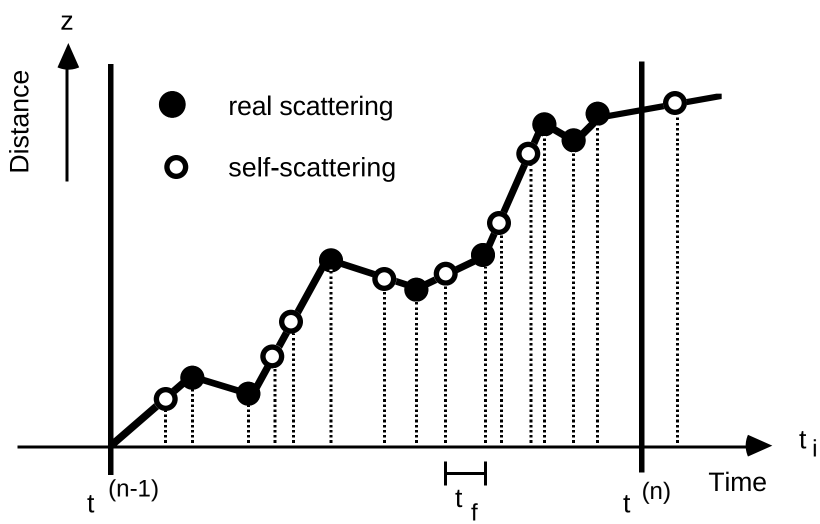
- The distribution of the states ($\mathbf{k}_i$, E_i) on a **k**-space grid becomes a representation of $f(\mathbf{k})$. An estimator is obtained from:

$$\langle A \rangle = \sum_{i=1}^{N_f} \frac{A(\mathbf{k}_i)}{N_f}$$

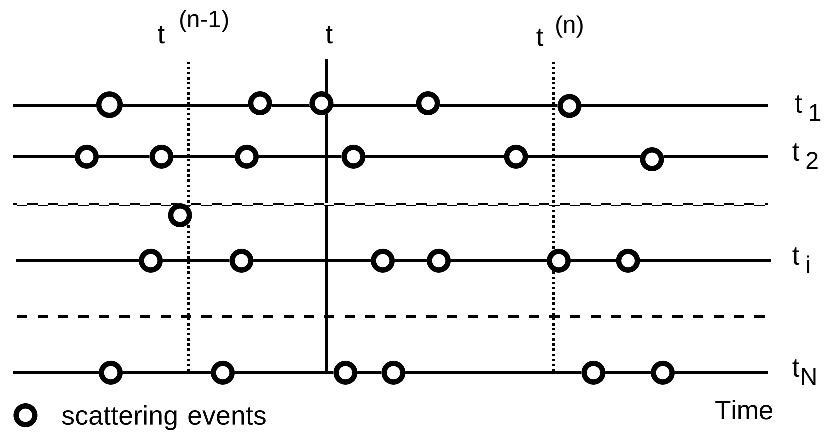
Visualizing the Monte Carlo Process



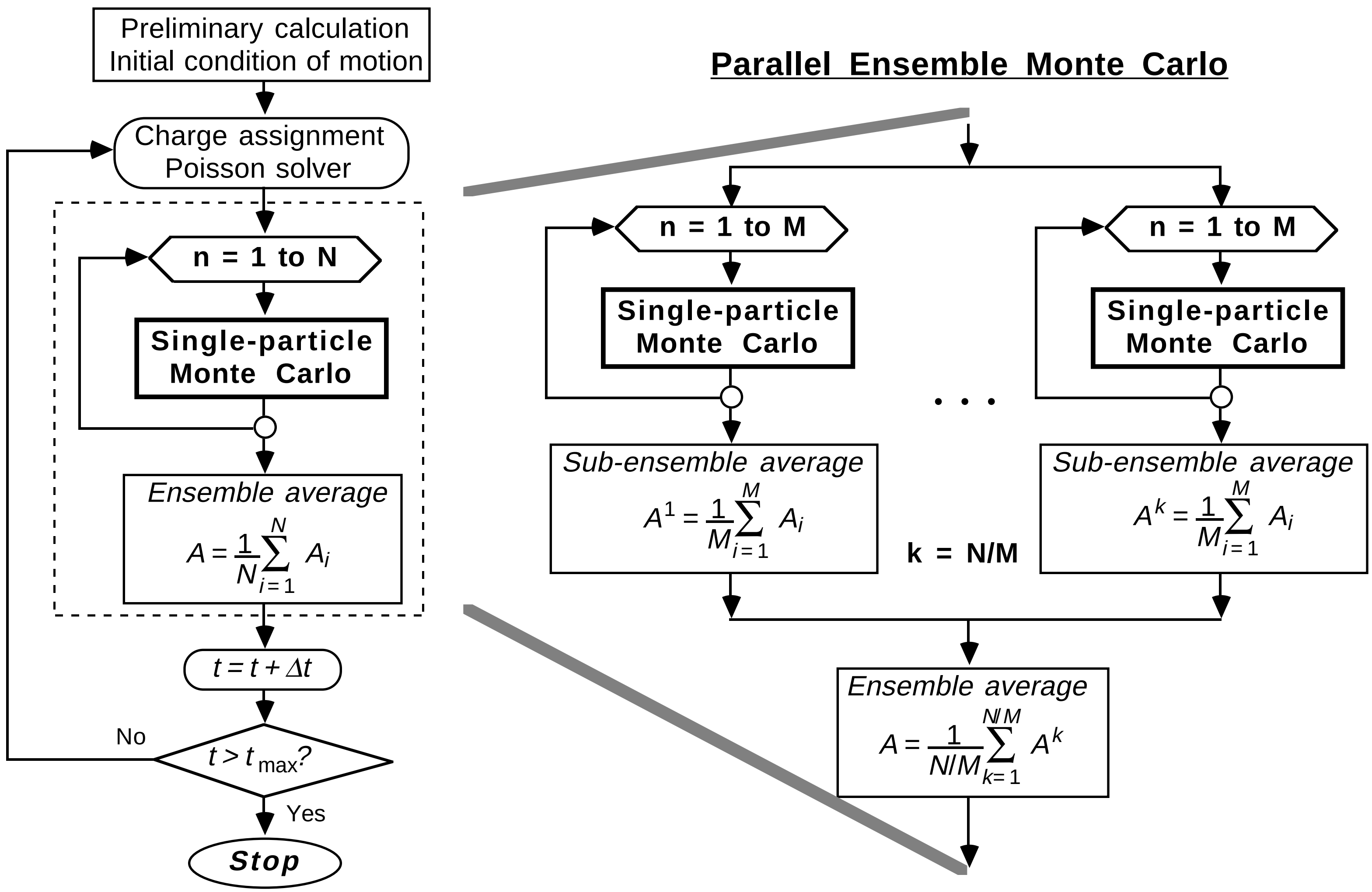
Free-flight — scattering — sampling



Synchronous-ensemble method



Sequential vs Parallel Monte Carlo Flowchart



Validity of Assumptions

❑ **Drift-diffusion formalism** — depends on the 1st moment of the BTE (e.g., μ, D)

- Quasi-thermal equilibrium: $T_e \approx T_L$
- Local-field approximation: $\mathbf{v}(\mathbf{r}) = \mu\mathcal{E}(\mathbf{r})$

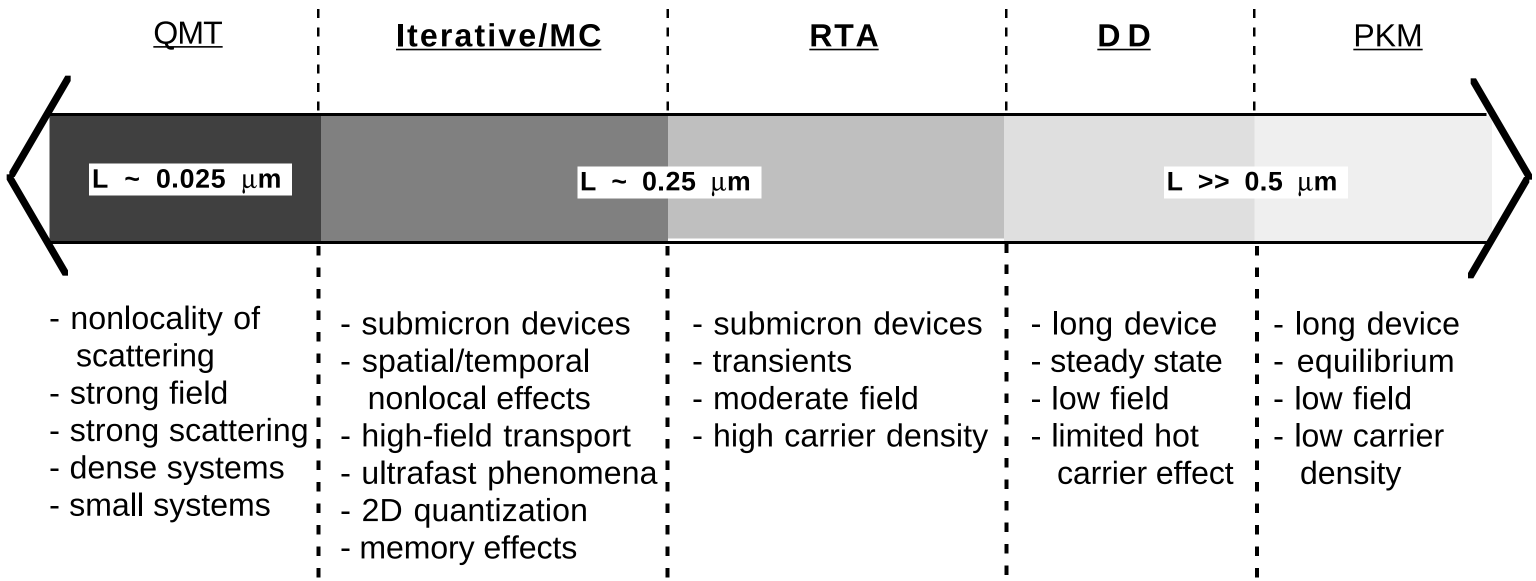
❑ **Relaxation-time approximation** — depends on the 2nd moment of the BTE (e.g., $\langle \mathbf{v} \rangle$, $\langle E \rangle$)

- Any perturbation of the distribution function, f, from the local equilibrium distribution, f_0, will relax back to f_0 within a "relaxation time" τ_R
- Valid when scattering is dominated by either isotropic or elastic mechanisms

❑ **Semiclassical transport theory (BTE)**

- "Instantaneous" collision: $\tau_c << \tau$
- "Frequent" scattering: $\tau << \tau_d$, $L > \Lambda$

Applications of the Semiclassical Transport Theory



- **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 syncronous
- **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 (μ, D, τ_m, τ_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 *a priori* assumption on the distribution function
  - Inherently parallel algorithm
- **Conclusion:** ***It won't be too long before the Monte Carlo approach to device simulation steps out of R&D labs and becomes a <u>routine</u> simulation tool***