

# Theory of the Monte Carlo Method for Semiconductor Device Simulation

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**Abstract**—A brief review of the semiclassical Monte Carlo (MC) method for semiconductor device simulation is given, covering the standard MC algorithms, variance reduction techniques, the self-consistent solution, and the physical semiconductor model. A link between physically based MC methods and the numerical method of MC integration is established. The integral representations the transient and the steady-state Boltzmann equations are presented as well as the corresponding conjugate equations. The structure of the iteration terms of the Neumann series and their evaluation by MC integration is discussed. Using this formal mathematical approach, the standard algorithms and variety of new algorithms are derived. The basic ideas of the weighted ensemble MC and the MC backward algorithms are explained.

**Index Terms**—Boltzmann transport equation, event biasing, Monte Carlo algorithms, semiconductor device simulation, small signal analysis.

## I. INTRODUCTION

OVER the last three decades the Monte Carlo (MC) method has evolved to a reliable and frequently used tool that has been successfully employed to investigate a great variety of transport phenomena in semiconductors and semiconductor devices.

The method consists of a simulation of the motion of charge carriers in the six-dimensional (6-D) phase space formed by the position and wave vectors. Subjected to the action of an external force, the pointlike carriers follow trajectories determined by Newton's law and the carrier's dispersion relation. Due to imperfections of the crystal lattice, the drift process is interrupted by scattering events, which are considered to be local in space and instantaneous in time. The duration of a drift process and the type of scattering mechanism are selected randomly according to given probabilities that describe the microscopic process.

In principle, such a procedure yields the carrier distribution in phase space. Integrating the distribution function over some phase space volume gives a measure for the relative number of carriers in that volume. Macroscopic quantities are obtained as mean values of the corresponding single-particle quantities. Moreover, the distribution function satisfies a Boltzmann equation (BE).

The method of generating sequences of drift and scattering appears so transparent from a physical point of view that it is frequently interpreted as a direct emulation of the physical process

rather than as a numerical method. The main MC algorithms used to date were originally devised from merely physical considerations, viewing an MC simulation as a simulated experiment. The proof that the used algorithms implicitly solve the BE was carried out later.

The alternative way to use the BE explicitly and to formulate MC algorithms for its solution was reported only one decade ago in the literature [1], [2]. New MC algorithms are derived which typically differ from the common ones by the fact that additional statistical variables appear, such as weights, that do not have a counterpart in the real statistical process.

## II. APPLICATION OF THE MC METHOD TO SEMICONDUCTOR DEVICES

Based upon the physical picture of the MC technique, it has been possible to apply the method to the simulation of a great variety of semiconductor devices. When the need for variance reduction techniques emerged, these have again been devised from physical considerations, such as splitting a particle into light ones by conserving the charge. For the MC simulation of devices, there are two algorithms generally employed, known as the *ensemble MC* (EMC) and the *one-particle MC* (OPMC) algorithms.

### A. MC Algorithms

For a systematic description of the MC algorithms, let us begin with the homogeneous case. Transient phenomena occur when the carrier system evolves from an initial to some final distribution. Accordingly, the evolution of an ensemble of test particles is simulated starting from a given initial condition. The physical characteristics are obtained in terms of ensemble averages, giving rise to the name "ensemble" MC [3], [4]. For example, the distribution function in a given phase space point at a given time is estimated by the relative number of particles in a small volume around the point.

The EMC algorithm can also be applied under stationary conditions. In this situation, for large evolution times the final distribution approaches a steady state, and the information introduced by the initial condition is lost entirely. Alternatively, the ergodicity of the process can be exploited to replace the ensemble average by a time average. Since it is sufficient to simulate one test particle for a long period of time, the algorithm is called "one-particle" MC. The effect of the particle's initial state vanishes for long simulation times. The distribution function in a given phase space point is estimated by the time spent by the particle in a fixed, small volume around the point divided by the total time the trajectory was followed. Another method of obtaining steady-state averages has been introduced by Price [5]. With the

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# Monte Carlo Method For Semiconductor Device Simulation The

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## **Monte Carlo Method For Semiconductor Device Simulation The:**

**The Monte Carlo Method for Semiconductor Device Simulation** Carlo Jacoboni, Paolo Lugli, 1989-10-30 This volume presents the application of the Monte Carlo method to the simulation of semiconductor devices reviewing the physics of transport in semiconductors followed by an introduction to the physics of semiconductor devices **Hierarchical Device Simulation** Christoph Jungemann, Bernd Meinerzhagen, 2012-12-06 This book summarizes the research of more than a decade Its early motivation dates back to the eighties and to the memorable talks Dr C Moglestue FHG Freiburg gave on his Monte Carlo solutions of the Boltzmann transport equation at the NASECODE conferences in Ireland At that time numerical semiconductor device modeling basically implied the application of the drift diffusion model On the one hand those talks clearly showed the potential of the Monte Carlo model for an accurate description of many important transport issues that cannot adequately be addressed by the drift diffusion approximation On the other hand they also clearly demonstrated that at that time only very few experts were able to extract useful results from a Monte Carlo simulator With this background Monte Carlo research activities were started in 1986 at the University of Aachen RWTH Aachen Germany Different to many other Monte Carlo research groups the Monte Carlo research in Aachen took place in an environment of active drift diffusion and hydrodynamic model development Monte Carlo Device Simulation Karl Hess, 2012-10-11 Monte Carlo simulation is now a well established method for studying semiconductor devices and is particularly well suited to highlighting physical mechanisms and exploring material properties Not surprisingly the more completely the material properties are built into the simulation up to and including the use of a full band structure the more powerful is the method Indeed it is now becoming increasingly clear that phenomena such as reliability related hot electron effects in MOSFETs cannot be understood satisfactorily without using full band Monte Carlo The IBM simulator DAMOCLES therefore represents a landmark of great significance DAMOCLES sums up the total of Monte Carlo device modeling experience of the past and reaches with its capabilities and opportunities into the distant future This book therefore begins with a description of the IBM simulator The second chapter gives an advanced introduction to the physical basis for Monte Carlo simulations and an outlook on why complex effects such as collisional broadening and intracollisional field effects can be important and how they can be included in the simulations References to more basic intro the book The third chapter ductory material can be found throughout describes a typical relationship of Monte Carlo simulations to experimental data and indicates a major difficulty the vast number of deformation potentials required to simulate transport throughout the entire Brillouin zone The fourth chapter addresses possible further extensions of the Monte Carlo approach and subtleties of the electron-electron interaction

**A Variance-reduced Electrothermal Monte Carlo Method for Semiconductor Device Simulation** Orazio Muscato, Vincenza Di Stefano, Wolfgang Wagner, 2012 *Monte Carlo Simulation of Semiconductor Devices* C. Moglestue, 2013-04-17 Particle simulation of semiconductor devices is a rather new field which has started to catch the

interest of the world's scientific community. It represents a time continuous solution of Boltzmann's transport equation or its quantum mechanical equivalent and the field equation without encountering the usual numerical problems associated with the direct solution. The technique is based on first physical principles by following in detail the transport histories of individual particles and gives a profound insight into the physics of semiconductor devices. The method can be applied to devices of any geometrical complexity and material composition. It yields an accurate description of the device which is not limited by the assumptions made behind the alternative drift diffusion and hydrodynamic models which represent approximate solutions to the transport equation. While the development of the particle modelling technique has been hampered in the past by the cost of computer time, today this should not be held against using a method which gives a profound physical insight into individual devices and can be used to predict the properties of devices not yet manufactured. Employed in this way it can save the developer much time and large sums of money, both important considerations for the laboratory which wants to keep abreast of the field of device research. Applying it to already existing electronic components may lead to novel ideas for their improvement. The Monte Carlo particle simulation technique is applicable to microelectronic components of any arbitrary shape and complexity.

**Springer Handbook of Semiconductor Devices** Massimo Rudan, Rossella Brunetti, Susanna Reggiani, 2022-11-10. This Springer Handbook comprehensively covers the topic of semiconductor devices embracing all aspects from theoretical background to fabrication modeling and applications. Nearly 100 leading scientists from industry and academia were selected to write the handbook's chapters which were conceived for professionals and practitioners: material scientists, physicists, and electrical engineers working at universities, industrial R & D, and manufacturers. Starting from the description of the relevant technological aspects and fabrication steps, the handbook proceeds with a section fully devoted to the main conventional semiconductor devices like e.g. bipolar transistors and MOS capacitors and transistors used in the production of the standard integrated circuits and the corresponding physical models. In the subsequent chapters, the scaling issues of the semiconductor device technology are addressed, followed by the description of novel concept based semiconductor devices. The last section illustrates the numerical simulation methods ranging from the fabrication processes to the device performances. Each chapter is self-contained and refers to related topics treated in other chapters when necessary, so that the reader interested in a specific subject can easily identify a personal reading path through the vast contents of the handbook.

**Physics of Semiconductor Devices** K. N. Bhat, A. Dasgupta, 2004. Contributed papers of the workshop held at IIT Madras in 2003.

**Stochastic Approaches to Electron Transport in Micro- and Nanostructures** Mihail Nedjalkov, Ivan Dimov, Siegfried Selberherr, 2021-04-05. The book serves as a synergistic link between the development of mathematical models and the emergence of stochastic Monte Carlo methods applied for the simulation of current transport in electronic devices. Regarding the models, the historical evolution path beginning from the classical charge carrier transport models for microelectronics to current quantum based nanoelectronics is explicatively followed. Accordingly, the

solution methods are elucidated from the early phenomenological single particle algorithms applicable for stationary homogeneous physical conditions up to the complex algorithms required for quantum transport based on particle generation and annihilation The book fills the gap between monographs focusing on the development of the theory and the physical aspects of models their application and their solution methods and monographs dealing with the purely theoretical approaches for finding stochastic solutions of Fredholm integral equations

**Frontiers In Electronics (With Cd-rom) - Proceedings Of The Wofe-04** Michael S Shur, Yoshi Nishi, Hiroshi Iwai, Hei Wong, 2006-08-10 Frontiers in Electronics reports on the most recent developments and future trends in the electronics and photonics industry The issues address CMOS SOI and wide band gap semiconductor technology terahertz technology and bioelectronics providing a unique interdisciplinary overview of the key emerging issues This volume accurately reflects the recent research and development trends from pure research to research and development and its contributors are leading experts in microelectronics nanoelectronics and nanophotonics from academia industry and government agencies

**GaN and Related Materials II** Stephen J. Pearton, 2000-10-31 The first GaN and Related Materials covered topics such as a historical survey of past research optical electrical and microstructural characterization theory of defects bulk crystal growth and performance of electronic and photonic devices This new volume updates old research where warranted and explores new areas such as UV detectors microw

**Compound Semiconductor Device Physics** Sandip Tiwari, 1992 This work provides a treatment of compound semiconductor device physics drawing upon low dimensional physics statistical methods and the use of one two and three dimensional analytical and numerical analysis techniques

*Multigrid Methods for Semiconductor Device Simulation* J. Molenaar, 1993

Parallel and Distributed Three-dimensional Monte Carlo Semiconductor Device Simulation Henry Sheng, Roberto Guerrieri, Alberto Sangiovanni-Vincentelli, 1995

*Numerical Simulation of Submicron Semiconductor Devices* Kazutaka Tomizawa, 1993-01-01 Describes the basic theory of carrier transport develops numerical algorithms used for transport problems or device simulations and presents real world examples of implementation

**International Conference on Simulation of Semiconductor Processes and Devices**, 2003

**Ultrafast Phenomena in Semiconductors**, 2002

*Hot Carrier Modeling in Metal-oxide-semiconductor Devices Using the Convective Scheme* Deborah Ann Fixel, 2007

**Simulation of Semiconductor Devices and Processes, Vol. 6** Heiner Ryssel, Peter Pichler, 1995 SISDEP 95 provides an international forum for the presentation of state of the art research and development results in the area of numerical process and device simulation Continuously shrinking device dimensions the use of new materials and advanced processing steps in the manufacturing of semiconductor devices require new and improved software The trend towards increasing complexity in structures and process technology demands advanced models describing all basic effects and sophisticated two and three dimensional tools for almost arbitrarily designed geometries The book contains the latest results obtained by scientists from more than 20 countries on process simulation and modeling simulation of process

equipment device modeling and simulation of novel devices power semiconductors and sensors on device simulation and parameter extraction for circuit models practical application of simulation numerical methods and software *IEICE Transactions on Communications, Electronics, Information, and Systems* ,1991 *Simulation of Semiconductor Devices and Processes, Vol. 3* Giorgio Baccarani,Massimo Rudan,1988

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