A theoretical analysis of this MC algorithm begins with the transformation of the stationary Boltzmann equation into an integral equation [4]. Because the obtained equation describes the evolution back in time and we are aiming at a forward MC algorithm, the conjugate equation needs to be formulated. The elements of the Neumann series of the conjugate equation are finally evaluated by means of MC integration [4]. Using this mathematically-based approach the Single-Particle MC method is derived in a formal way. For the first time, the independent, identically distributed random variables of the simulated process are identified, allowing to supplement this MC method with the natural stochastic error estimate. Furthermore, the extension of the MC estimators to the case of biased events is derived.

The kernel of the conjugate equation yields the natural probability distributions which are used for the construction of the particle trajectory. However, it is possible to choose other than the natural probabilities for the MC integration of the terms of the Neumann series. In that case one constructs numerical trajectories that differ from the physical ones. The motivation for using arbitrary probabilities is the possibility to guide particles towards a phase space regions of interest to enhance statistics. In this work we increase carrier diffusion against a retarding electric field by introducing artificial carrier heating. The probability for phonon absorption is increased at the expense of phonon emission, a measure which increases the probability of a numerical particle to surmount an energy barrier. In regions with small field, where transport is diffusion dominated, the distribution of the scattering

\[1\]

This work has been partly supported by the IST program, project NANOTCAD, IST-1999-10828.
angle is biased so as to induce artificial carrier diffusion. Furthermore, the distribution at
the boundaries has been modified, injecting test particles at much higher temperature than
the lattice temperature.

Changing probability distributions requires compensatory changes in the estimators. The
event bias technique can be summarized by a simple rule. Whenever in the course of nu-
merical trajectory construction a random variable, for example, a free flight time or an after
scattering state, is selected from a numerical density rather than from a physical density, the
weight of the test particle changes by the ratio of the physical over the numerical density.
As a consequence, the weight of a test particle evolves randomly. Individual particle weights
can evolve to extremely different values, predominantly to very small ones.

Optimal values of the parameters which control the bias are not known a priori. If the bias
is chosen too small, not enough particles will, for example, surmount an barrier, rendering
statistical enhancement inefficient. On the other hand, by choosing the bias too large nu-
merous numerical trajectories will pass through the low concentration region. However, due
to the aggressive biasing the spreading of the particle weights will be very large, and the
recorded averages will again show a large variance. To find some optimum between these
two extreme cases a careful tuning of the bias parameters is necessary.

The described behavior of the event bias scheme suggests the usage of additional variance
reduction techniques [5]. In the presented simulation study evolution of the particle weight
is governed predominantly by the event bias technique, and explicit measures are taken only
to prevent particle weights from getting extremely high or low [6].

The formal approach, which is based on Monte Carlo integration of the terms of the Neu-
mann series, clearly shows what the independent, identically distributed random variables
are. A realization of such random variable is a complete numerical trajectory that starts
and terminates at the domain boundary. Only complete numerical trajectories can be con-
sidered independent from each other, whereas particle states generated on one trajectory
are statistically dependent. Knowing these random variables standard textbook formulae
can be applied to estimate the variance of the MC estimates [7].

References

