Monte Carlo Algorithm for Nanoscale Electro-Thermal Optimization

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ABSTRACT

In this paper, we are presenting a Monte Carlo method based algorithm selected for electro-thermal optimization in nanoelectronics devices. We consider that we must be able to know the position of electrons for modeling thermal phenomena of such devices. For this, we define the governing equation from which we will be able to do so. This equation is the Schrödinger equation but in addition we are considering the Boltzmann Transport Equation as well. We are aware that we can't know for sure the position of an electron, but these equations will give us the probability of their position. The model of nanoelectronics devices is simplified. Each heat source is approximated by Dirac's distribution. The optimal location of the heat sources in nonoscale devices is searched by some optimization rules in conjunction with a specific Monte Carlo method. This optimization can be generalized for any system containing a number *N* of nanoelectronics elements.

Keywords: electro-thermal, optimization, Monte Carlo method, algorithm, nanoelectronics

1 INTRODUCTION

In our previous works we optimized thermal fields in macro- and micro- system containing several numbers of electronic components [1], [2]. At those scales, electro-thermal-phenomena are very important to be considering in the overall design process.

However, heat phenomena at the nanoscale differ largely from those at micro- and macro-scales. This is not surprising because we know that the classical laws of physics are no more applicable to explain various phenomena at the nanoscale level, thus we must use the quantum physics. So this is the same case for nanoscale electro-thermal phenomena.

2 EQUATIONS

The Schrödinger equation for the Kohn-Sham single electron states reads by the following equation:

$$-\frac{\hbar^2}{2}\nabla\left[m^{-1}(r)\nabla\psi(r)\right]+V(r)\psi(r)=E\psi(r) \qquad (1)$$

Where $\hbar$ is the reduced Planck's constant, m is the effective mass tensor, and ψ and E are the eigenfunctions and eigenvalues respectively.

The BTE (Boltzmann Transport Equation) for a phonon mode i under a temperature gradient ∇T is given by:

$$-Vg,i.\nabla T\frac{\partial n_i}{\partial T}+(\frac{\partial n_i}{\partial T})=0 \qquad (2)$$

Where n_i is the phonon mode occupation number, t is the time, and V_{gi} is the phonon group velocity, defined as $\partial\omega/\partial k$, where ω is the angular frequency and k is the wave vector. The solution of this equation describes the steady-state distribution of phonons in a system, and how that distribution comes about through the effects of diffusion (first term) and scattering (second term, also known as the collision term).

3 OPTIMIZATION RULES

Generally, optimization can be performed for any system containing a number *N* of nanoscale heat sources. Every localized heat source in this system is modeled by a separate Dirac's distribution [3].

The system composed by *N* nanoelectronic elements approximated by a Dirac's distribution can be unequivocally described by vectors **C** and **Q**. The components of vector **C** are coordinates x_k and y_k of the

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successive Dirac's distributions, defined in the space of real numbers

$$\mathbf{C} = [x_1, y_1, x_2, y_2, ..., x_k, y_k, ..., x_N, y_N] \quad (3)$$

Regarding the finite dimensions of the analyzed system, related components of vector **C** must be submitted to the limitations

$$(x_k \in \boldsymbol{R}) \cap [x_k \in (-a, a)] \cap (y_k \in \boldsymbol{R}) \cap [y_k \in (-b, b)] \quad (4)$$

The components of vector **Q** are the values of the linear heat sources generating rate q_k inside of every analyzed element. The value of the linear heat sources generating rate q_k is related to the power losses P_k in each element as follows

$$\mathbf{Q} = [q_1, q_2, ..., q_k, ..., q_N] = \left[\frac{P_1}{z_1}, \frac{P_2}{z_2}, ..., \frac{P_k}{z_k}, ..., \frac{P_N}{z_N} \right] \quad (5)$$

Simplifying analysis to the 2D model description in the plan *XY*, we must also consider the influence of both the semiconductor junction structure and the dimension through the *Z* axis for the q_k value. From this point of view, values z_1, z_2,..., z_k in equation (5) describe the dimension of the heat generation area through the *Z* axis as well as the dimension for each analyzed element, which can be also, considered a subsystem.

Optimization for the overall structure of the system is performed in conformity with the temperature minimization criteria in the chosen areas of the system. Regarding others non unexpected modifications of the optimization algorithm, we introduce a modified complex objective function [2]

$$\|T\|_C = round\left(\sum_{k=1}^{N} a_k \|T\|_{Ck} \right) \quad (6)$$

The value of a global norm $||T||_C$ is built on the bases of the discretized real values of local norms $||T||_{Ck}$, determined separately for each element

$$\|T\|_{Ck} = \sum_{u=1}^{DL} \boldsymbol{1}\left(T_{E,u} - \|T\|_{\infty,k} \right) \quad (7)$$

A local norm $||T||_{Ck}$ is calculated as an addition of the Heaviside functions. The argument of the Haeviside function is the difference between the edge value T_E and a calculated maximal temperature value in the analyzed electronics element $\|T\|_{\infty,k}$. The edge values T_E introduced in equation (7) are naturally ranged in increasing order inside of the arbitrarily defined sub-space of the real numbers. The maximal temperature value $\|T\|_{\infty,k}$ in the analyzed element is determined on the basis of the temperature values calculated in the points of the discretized space *XY* situated close to the Dirac's distribution. In this way, we can make an appropriate evaluation of the temperature of the semiconductor junction – the most critical point for temperature increase and introduce it to the optimization procedure.

The definition of the composed norm (6) requires the introduction of the vector of weight coefficients

$$\mathbf{A} = [a_1, a_2, ..., a_k, ..., a_N] = \left[\frac{P_1}{P_C}, \frac{P_2}{P_C}, ..., \frac{P_k}{P_C}, ..., \frac{P_N}{P_C} \right] \quad (8)$$

The factors values are determined by power losses P_k in the analyzed element. P_C represents the total amount of power losses in the system.

Based on the target function definition (6), we can determine the optimal displacement of a system's elements as one of the analyzed variants of vector **C**

$$\|T\|_{C,l} = \min\left\{ \|T\|_{C,1}, ..., \|T\|_{C,l}, ..., \|T\|_{C,M} \right\} \Rightarrow (\mathbf{C}_{OPT} = \mathbf{C}_l) \quad (9)$$

where *M* represents a number of the system's variants calculated with the optimization algorithm rules.

4 MONTE CARLO ALGORITHM

Monte Carlo simulations use random moves to explore the search space to find out some information about the space. In a simple Monte Carlo simulation, all random moves are accepted such that a different region of search space is sampled at each step. In 1953, Nicholas Metropolis and coworkers [4] proposed a new sampling procedure which incorporates a *temperature* of the system. This is done so that the Boltzmann average of a property of the system can be easily calculated. This modified Monte Carlo method is known as a Metropolis Monte Carlo simulation. As presnted in reference [5], Metropolis method configurations are generated form a previous state using a transition probability which depends on the energy difference between the initial and final states. The sequence of states produced follows a time ordered path, but the time in this case is reffered to as "Monte Carlo time" and is non-deterministic. (This can be seen from an evaluation of the commutator of the Hamiltonian and an arbitrary spin; the value, which gives the time dependence of the spin, is zero). For relaxational models, such as the Ising model, the time-dependent behavior is described by a master equation:

$$\frac{\partial P_n(t)}{\partial t} = -\sum_{n \neq m} [P_n(t) W_{n \to m} - P_m(t) W_{m \to n}] \quad (10)$$

where $P_n(t)$ is the probability of the system being in state n at time t, and $W_{n\to m}$ is the transition rate for n→m. In equilibrium $\partial P_n(t)/\partial t = 0$ and the terms of the right-hand side of Eqn. (10) must be equal. The resultant expression is know as "detailed balance":

$$P_n(t)\, W_{n\to m} = P_m(t)\, W_{m\to n} \qquad (11)$$

The probability of the nth state occurring in a classical system is given by

$$P_n(t) = e^{-E_n / k_B T} / Z \qquad (12)$$

where Z is the partition function. This probability is usually not exactly known because of the denominator; however, one can avoid this difficulty by generating a Markov chain of states, i.e. generate each new state directly from the preceding state. If we produce the *n*th state from the *m*th state, the relative probability is the ratio of the individual probabilities and the denominator cancels. As a result, only the energy difference between the two states is needed

$$\Delta E = E_n - E_m \qquad (13)$$

Any transition rate which satisfies detailed balance is acceptable. The first choice of rate which was used in statistical physics is the Metropolis form [4]

$$W_{n\to m} = \tau_0^{-1} \exp(-\Delta E / k_B T)\,, \quad \Delta E > 0 \qquad (14)$$

$$= \tau_0^{-1}\,, \qquad \Delta E < 0 \qquad (15)$$

where τ_0 is the time required to attempt a spin-flip. (Often this "time unit" is set equal o unity and hence spressed in the equations). The way the Metropolis algorithm is implemented can be described by a simple recipe [5]:

(1) Choose an initial state
(2) Choose a site *i*
(3) Calculate the energy change ΔE which results if the spin at site is overturned
(4) Generate a random number *r* such that $0 < r < 1$
(5) If $r < \exp(-\Delta E/k_B T)$, flip the spin
(6) Go the next site and go to (3)

After a set of number of spins have been considered, the properties of the system are determined and added to the statistical average which is being kept. Note that the random number *r* must be chosen *uniformly* in the interval [0,1], and successive random numbers should be uncorrelated. The "standard" mesure of Monte Carlo time is the Monte Carlo step/site (MCS/site) which corresponds to the consideration of every spin in the system once. With this algorithm states are generated with a probability proportional to Eqn. (12) once the number of states is sufficiently large that the initial transients are negligible. Then, the desired averages $(A) = \sum_n P_n A_n$ of a variable A simply become arithmetic averages over the entire sample of states which is kept. Note that if an attempted spin-flip is rejected, the old state is counted again for the averaging.

5 CONCLUSION AND FUTURE WORK

We have presented an exploratory attempt of possible formulation for electro-thermal analysis in nanoelectronics devices. In fact, we are assembling a Schrödinger equation, our previously developed optimization criteria and selected description of a specific Monte Carlo algorithm.

From our analysis, it's seems be very appropriate to apply both the statistical physics and optimizations methods for optimal temperature fields determination in the nanoelecronics systems manufacturing processes and that as the scientific answer for an immediate industrial demand.

The next step in this research will be to synthesize an appropriate routine and implement it in the high performance computing environment. The results of the simulations runs and models validations will follow in the near future.

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