# A GLOBALLY CONVERGENT METHOD FOR SOLVING ENERGY BALANCE EQUATIONS

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**Abstract**

A new globally convergent method for solving the energy balance equation is developed. The original energy balance equation is re-expressed as an energy-flux continuity equation which is similar to the current continuity equation. A new Slotboom-like variable for electron temperature is introduced. The new expression for the energy balance equation is then discretized using a method which is similar to the Scharfetter-Gummel scheme. The discretization provides a system of linear difference equations whose coefficient matrix is diagonally dominant. In addition to converging for any initial guess, this method avoids having to solve large matrix equations by decoupling the system through the use of iterative solution techniques. This decoupling significantly reduces memory requirements and facilitates parallel computation, thereby making the new method attractive for 3-D applications.

## I. Introduction

Energy Transport (ET) simulations have traditionally been plagued by convergence and stability problems. A major source of these difficulties has its origin in the energy balance equation. The difficulties arise because electron temperature may vary very rapidly between mesh points. Much work has been devoted toward improving these computational difficulties[1,2,3]. The first significant contribution towards overcoming these numerical difficulties used a Scharfetter-Gummel-like discretization of the ET model[1]. While this approach significantly advanced the state of the art, convergence and stability difficulties remain. Our new method overcomes many of the numerical problems associated with energy balance equations. With the new method, we use exponential fitting to resolve the rapid variation in electron temperature $T_e$ that occurs between grid points. Additionally, instead of the usual discretization in terms of $T_e$, we have devised a new discretization which is with respect to a Slotboom-like variable. This discretization provides a linear form for the discretized energy balance equation. The matrix associated with this discretized equation is guaranteed to be diagonally dominant. By solving the diagonally dominant matrix equation using iterative methods, the convergence of the energy balance equation is guaranteed. In addition to being globally convergent, the new method requires little memory, and is well-suited for parallel computation.

## II. Model Description

We start with the energy balance equation for electrons presented by Blotekjaer[4]:

$$\frac{\partial W}{\partial t} + \nabla \cdot (\vec{v}_d W) = -qn\vec{v}_d \cdot \vec{E} - \nabla \cdot (\vec{v}_d n k_B T_e) - \nabla \cdot \vec{Q} + \left(\frac{\partial W}{\partial t}\right)_c \tag{1}$$

where $W$ is the average energy density; $\vec{v}_d$ is the drift velocity; $n$ is the electron concentration; $\vec{E}$ is the electric field; $k_B$ is Boltzmann's constant; $T_e$ is the electron temperature; and $\vec{Q}$ is the heat flux; $\left(\frac{\partial W}{\partial t}\right)_c$ is the rate of energy loss due to collisions with the lattice.

Next, typical approximations are made:

(1) The energy density is approximated by the random energy only:

$$W \approx \frac{3}{2} n k_B T_e \tag{2}$$

(2) The collision term is evaluated using the relaxation time approximation:

$$\left(\frac{\partial W}{\partial t}\right)_c = -\frac{W - W_o}{\tau_W(T_e)} \tag{3}$$

where $\tau_W(T_e)$ is the energy relaxation time, and $W_o$ is the average energy density in thermal equilibrium.
(3) The heat flux is expressed by

$$\vec{Q} = -\kappa_c \bigtriangledown T_e \tag{4}$$

where $\kappa_c$ is the electron thermal conductivity.

### III. Formulation of the Energy Balance Equation

To derive a globally convergent form of Eqn.(1), we parallel a state of the art technique which was developed for the drift-diffusion model[5]. First, using the above approximations, we can rewrite Eqn.(1) in the energy flux continuity form:

$$\bigtriangledown \cdot \vec{S} = \vec{J}_n \cdot \vec{E} - n\frac{\frac{3}{2}k_B T_e - \frac{3}{2}k_B T_L}{\tau_\omega(T_e)} \tag{5}$$

where $\vec{S}$ is the energy flux:

$$\vec{S} = \frac{\vec{J}_n}{-q}\frac{5}{2}k_B T_e - \kappa_c \bigtriangledown T_e \tag{6}$$

Eqn. (5) looks very similar to the current continuity equation in the DD model. Eqn. (6) shows that the energy flow $\vec{S}$ consists of "drift energy flux" and "diffusion energy flux," and is similar to the current equation in the DD model.

Now, we express $T_e$ in terms of a new Slotboom-like variable $g$:

$$T_e = g\exp(\psi_n/a_T) \tag{7}$$

where $\psi_n$ is the electron quasi-Fermi potential, and $a_T$ is constant

$$a_T = \frac{\kappa_c}{\frac{5}{2}\mu_n n k_B} = 0.0207V \tag{8}$$

Rewriting the energy flux $\vec{S}$ in terms of the Slotboom-like variable $g$, we obtain:

$$\vec{S} = -\kappa_c \exp(\psi_n/a_T) \bigtriangledown g \tag{9}$$

Finally, by substituting $\vec{S}$ into the steady-state energy balance equation, we can rewrite the steady-state energy balance equation with the variable $g$ in the self-adjoint form:

$$\bigtriangledown \cdot (-\kappa_c \exp(\psi_n/a_T) \bigtriangledown g) = \vec{J}_n \cdot \vec{E} - \frac{ng\exp(\psi_n/a_T) - W_o}{\tau_W(T_e)} \tag{10}$$

In order to analyze characteristics of the energy balance equation, Eqn.(10) can be expressed in 1-D case as follows:

$$\frac{d^2g}{dx^2} + \frac{1}{a_T}\frac{d\psi_n}{dx}\frac{dg}{dx} = \frac{\vec{J}_n \cdot \vec{E} - n\frac{g\exp(\psi_n/a_T) - \omega_o}{\tau_\omega(T_e)}}{-\kappa_c \exp(\psi_n/a_T)} \tag{11}$$

It is easy to show that Eqn.(11) is singularly perturbed, and thus rapidly varying, due to the fact that in general the coefficient of $(dg/dx)$ is very large compared to the coefficient of $(d^2g/dx^2)$. Furthermore, the solution of Eqn.(11) contains an exponential form implying the exponential variation of $T_e$ between mesh points.

## IV. Discretization of the Energy Balance Equation

In order to resolve the rapid variation of $T_e$, we employ a Scharfetter-Gummel-like method to discretize the energy balance equation in terms of the variable $g$. Here $S$ parallels the role of the current density $J$ of the drift-diffusion model, and we thus take the energy flux $S$ to be constant between mesh points. Applying finite differences to Eqn. (10) then yields the following discretized energy balance equation:

$$\frac{2}{h_i + h_{i-1}}\left[\kappa_c\,|_{i+\frac{1}{2},j}\,\frac{\exp(\psi_{ni,j}/a_T)}{h_i}B\left(\frac{\psi_{ni,j}-\psi_{ni+1,j}}{a_T}\right)(g_{i+1,j}-g_{i,j})\right.$$
$$\left.+\kappa_c\,|_{i-\frac{1}{2},j}\,\frac{\exp(\psi_{ni,j}/a_T)}{h_{i-1}}\times B\left(\frac{\psi_{ni,j}-\psi_{ni-1,j}}{a_T}\right)(g_{i-1,j}-g_{i,j})\right]$$
$$\frac{2}{k_i + k_{i-1}}\left[\kappa_c\,|_{i,j+\frac{1}{2}}\,\frac{\exp(\psi_{ni,j}/a_T)}{k_j}B\left(\frac{\psi_{ni,j}-\psi_{ni,j+1}}{a_T}\right)(g_{i,j+1}-g_{i,j})\right.$$
$$\left.+\kappa_c\,|_{i,j-\frac{1}{2}}\,\frac{\exp(\psi_{ni,j}/a_T)}{k_{j-1}}\times B\left(\frac{\psi_{ni,j}-\psi_{ni,j-1}}{a_T}\right)(g_{i,j-1}-g_{i,j})\right]$$
$$=\frac{\frac{3}{2}k_B n_{i,j}g_{i,j}\exp(\psi_{ni,j}/a_T)-W_o}{\tau_W(T_{ei,j})}-\vec{J}_{ni,j}\cdot\vec{E}_{i,j} \tag{12}$$

where B(x) is the Bernoulli function

$$B(x)=\frac{x}{\exp(x)-1} \tag{13}$$

The convergence of the above system of equations is guaranteed, and the energy balance equation can be solved no matter the initial guess. To see that the convergence is indeed global, one can observe that the above matrix will always be diagonally dominant. Since this matrix is diagonally dominant, global convergence is guaranteed when the iterative solution techniques, such as the Jacobi, Gauss-Seidel or SOR methods, are employed. Substituting $g_{i,j}$ back to Eqn. (7), electron temperature $T_{ei,j}$ can be obtained.

## V. Results

To test the technique, we generated initial guesses using a random function:

$$T_e^{(0)}(i,j)=r(i,j)\times 2000K, \quad (0<r<1) \tag{14}$$

where $r(i,j)$ is a random number[6]. We solved the energy balance equation for a MOSFET. For different runs, we generated different random initial guesses. For each trial, it took less than 20 iterative loops to obtain exactly the same results using the convergence criterion:

$$Max_{i,j}\left(\frac{T_e^{(n+1)}(i,j)-T_e^{(n)}(i,j)}{T_e^{(n)}(i,j)}\right)<10^{-5} \tag{15}$$

Fig. 1 shows the result of a computation performed for a MOSFET in the steady state. Fig. 2 shows that this method of solving the energy balance equation gives values for average energy that agree well with Monte Carlo calculations, which used the same collision mechanisms.

## VI. Conclusions

We have developed a globally convergent method for solving energy balance equations. The method represents a first step in facilitating the convergence of hydrodynamic simulators in general. Finally, by using an iterative approach, the method also has the advantages that it requires very little memory and lends itself very well for parallel computation, making it attractive for 3-D applications.

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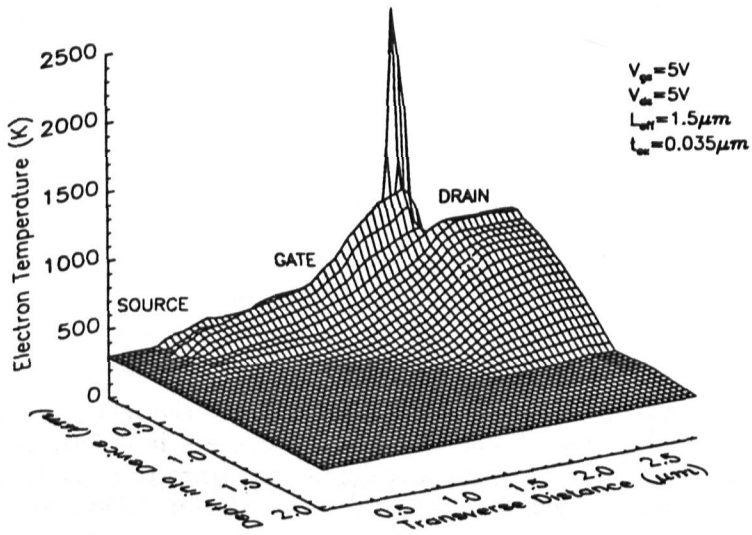


Fig.1 Electron Temperature Distribution in MOSFET

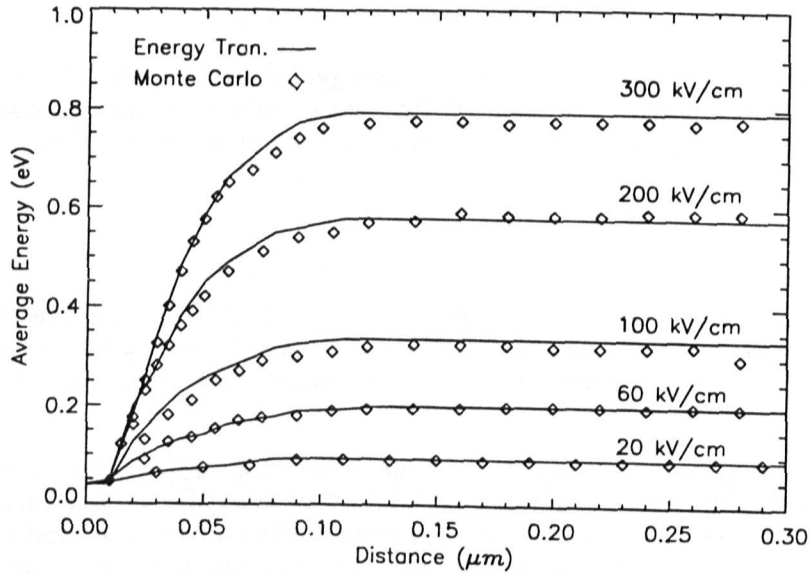


Fig.2 Average Energy vs Distance for Homogeneous Field