An Efficient Decoupled Algorithm for Solving Energy Transport Equations

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Introduction

The energy transport (ET) model is now indispensable to simulate deep-submicron semiconductor device characteristics [1], and the issue of how to solve the ET equations is still of great importance. Either the Newton algorithm [2] [3] or the decoupled algorithm [4] is currently used. With the Newton algorithm, large memory capacity is required and, in addition, it is necessary to start with a good initial guess to ensure stable convergence. Thus the decoupled algorithm will remain a convenient scheme, provided its slow convergence is improved. The purpose of this study is to propose a very simple and efficient way to improve convergence of the decoupled algorithm. First, the iterative process in each equation solver has been discarded; this enables to avoid the convergence problem of the energy balance (EB) equation solver and also leads to the decrease in CPU-time. Next, the Jacobian matrix of the EB equation has been altered to provide a 'reduced' Jacobian matrix, which improves the convergence speed.

Simple and efficient decoupled algorithm

The ET model recently proposed by [3] has been incorporated in our device simulator DS2 (Nippondenso Semiconductor Device Simulator) [5]. This model gives the following discretized EB eq. for ith box:

$$Q_i \equiv -\sum_{j\neq i} qC_e \frac{d_{ij}}{L_{ij}} [\, B(\tilde{u}_{ij})\, n_j\, \mu_j\, \tilde{T}_j^2 - B(-\tilde{u}_{ij})\, n_i\, \mu_i\, \tilde{T}_i^2 \,] - \langle F \cdot J \rangle_i\, \Omega_i + \frac{3}{2} qn_i \frac{\tilde{T}_i - \tilde{T}_0}{\tau_w} \Omega_i = 0. \tag{1}$$

The inner product term $\langle F \cdot J \rangle_i$ is discretized as follows:

$$\langle F \cdot J \rangle_i\, \Omega_i = \sum_{j\neq i} \frac{\psi_i - \psi_j}{L_{ij}} J_{ij} \frac{L_{ij} d_{ij}}{2} \quad ; \quad J_{ij} = \frac{q}{L_{ij}} [\, B(\tilde{u}_{ij})\, n_j\, \mu_j\, \tilde{T}_j - B(-\tilde{u}_{ij})\, n_i\, \mu_i\, \tilde{T}_i \,]. \tag{2}$$

Figure 1 shows the conventional decoupled algorithm; Poisson's eq. and the carrier-continuity eq. (drift-diffusion (DD) eqs.) are solved simultaneously by Newton method. In MOS simulations, the EB eq. solver sometimes fails to converge unless a small voltage step (<0.1V) is given. First, the iterative process in EB eq. solver has been discarded to avoid this problem. It can be shown that it does not exacerbate convergence speed. Furthermore, even the Newton iteration in DD eq. solver is unnecessary, though it is absolutely necessary at the first step just after the bias voltage is stepped. Figure 2 shows the resulting simple decoupled algorithm.

Convergence behavior was examined for a 1-dimensional *pn* diode (Fig. 3) and for an n-channel MOSFET with Leff = 0.35μm (Fig. 4). In the *pn* diode simulation, the reverse bias voltage was stepped from 3V to 4V. In the MOSFET simulation, the gate voltage was stepped from 1.8V to 2.0V with Vd = 3V. The maximum temperature updates in eV are plotted in these figures. The circles show the convergence of the conventional decoupled algorithm and the triangles show the convergence when the iterative processes are discarded. There is little difference between these two cases; therefore, it is concluded that the iterative processes in both the solvers are unnecessary. This simplification also leads to the reduction in iteration number and, consequently, in CPU-time.

On the other hand, the convergence rate is still low. Next, a method to improve the convergence will be proposed.

With the exact Jacobian matrix of the EB eq., the temperature updates tend to be underestimated; this contributes to the slow convergence speed. Conversely, with a 'reduced' Jacobian matrix calculated by assuming $\tilde{u}_{ij}$ and $\mu_k \tilde{T}_k$ are constant, the temperature updates tend to be overestimated; the temperature converges with oscillation of large amplitude. This large oscillation is attributed to the oscillation of the inner product term $\langle F \cdot J \rangle_i$. Thus it is expected that convergence will be improved by appropriately including the temperature derivative of $\langle F \cdot J \rangle_i$ in the reduced Jacobian matrix.

The following is the reduced Jacobian matrix employed:

$$\frac{\partial Q_i}{\partial \tilde{T}_i} = \sum_{j\neq i} qC_e \frac{d_{ij}}{L_{ij}} B(-\tilde{u}_{ij})\, n_i\, \mu_i\, \tilde{T}_i - \delta \sum_{j\neq i} \frac{\psi_i - \psi_j}{L_{ij}} \Delta_{ij} \frac{L_{ij} d_{ij}}{2} + \frac{3qn_i}{2\tau_w} \Omega_i$$

$$\frac{\partial Q_i}{\partial \tilde{T}_{j\,(j\neq i)}} = -qC_e \frac{d_{ij}}{L_{ij}} B(\tilde{u}_{ij})\, n_j\, \mu_j\, \tilde{T}_j - \delta \frac{\psi_i - \psi_j}{L_{ij}} \Delta_{ij} \frac{L_{ij} d_{ij}}{2} \tag{3}$$

$$\text{where} \quad \Delta_{ij} \equiv \frac{q}{L_{ij}} [\, B'(\tilde{u}_{ij})\, n_j\, \mu_j\, \tilde{T}_j + B'(-\tilde{u}_{ij})\, n_i\, \mu_i\, \tilde{T}_i \,] \frac{\partial \tilde{u}_{ij}}{\partial \tilde{T}_i}.$$

The adjustment parameter δ, which affects whether the temperature updates are underestimated or overestimated, is chosen to be 0.4. The squares in Fig. 3 and Fig. 4 show the convergence when this reduced Jacobian matrix is used. In the *pn* diode simulation, the iteration number decreases nearly two-thirds. Convergence is also improved in the MOSFET simulation, but it slows down below 10^{-3} in this case. Ad hoc adjustment of δ is still necessary to obtain a convergence below 10^{-5}.

In spite of its simplicity, this decoupled algorithm utilizing the reduced Jacobian matrix is an efficient way to solve the ET equations. It can be directly applied to another model equation and provide good convergence.

Conclusion

A simple and efficient decoupled algorithm for solving ET equations has been proposed. First, the iterative process in each equation solver has been discarded. Next, the reduced Jacobian matrix has been employed to obtain better convergence. In the *pn* diode simulation, the iteration number decreases nearly two-thirds. It is concluded that, though very simple, this algorithm is efficient in improving the capability of the device simulator taking account of the ET model.

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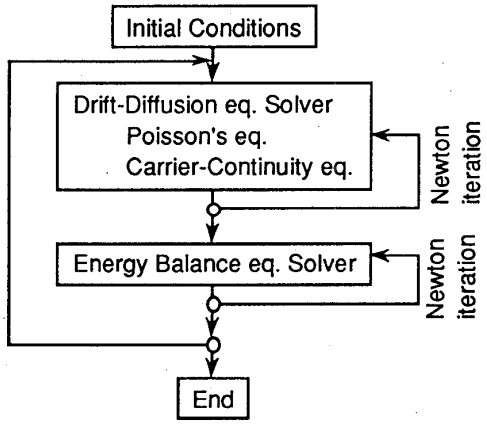

Fig. 1. The conventional decoupled algorithm.

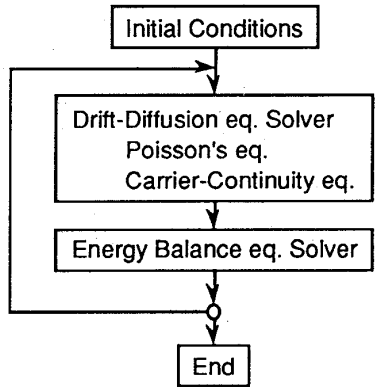

Fig. 2. The simple decoupled algorithm without the iterative processes.

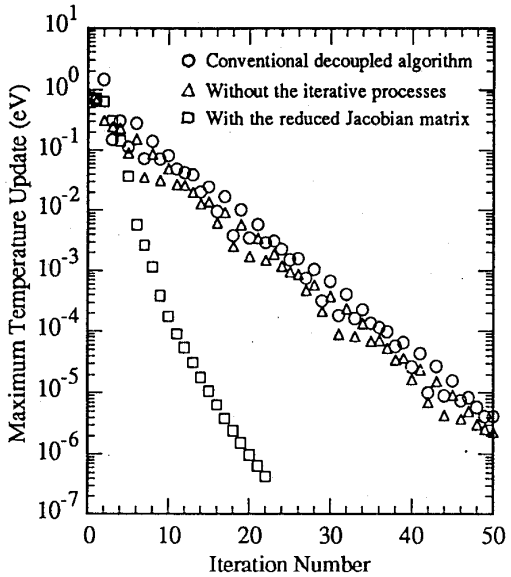

Fig. 3. Convergence for a 1-dimensional *pn* diode. The reverse bias is stepped from 3V to 4V.

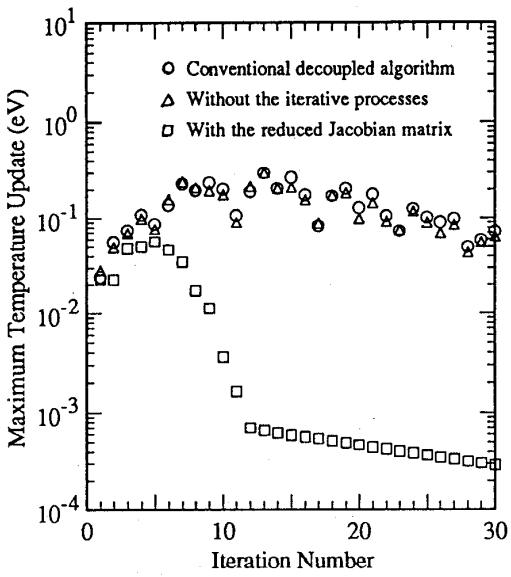

Fig. 4. Convergence for an n-channel MOSFET The gate voltage is stepped from 1.8V to 2.0V.