Interconnect Thermal Simulation with Higher Order Spatial Accuracy

Yijiang Shen, Ngai Wong and Edmund Y. Lam
Department of Electrical and Electronic Engineering
The University of Hong Kong, Pokfulam Road, Hong Kong
E-mail: {yjshen, nwong, elam}@eee.hku.hk

***Abstract*— This paper reports on a numerical analysis of interconnect thermal profile with fourth-order accuracy in space. The interconnect thermal simulation is described in a partial differential equation (PDE), and solved by finite difference time domain (FDTD) techniques using a fourth-order approximation of the spatial partial derivative in the PDE. A recently developed numerically stable algorithm for inversion of block tridiagonal and banded matrices is applied when the thermal simulation is conducted using Crank-Nicolson method with fourth-order spatial accuracy. We have promising simulation results, showing that the proposed method can have more accurate temperature profile before reaching the steady state than the traditional menthols and the runtime is linearly proportional to the number of nodes.**

I. Introduction

Due to rapid increase of power and packaging densities in recent years, a great deal of attention has been paid to thermal issues on the reliability and performance for very large scale integration (VLSI) design and manufacturing. More and more efforts have been put in the development of numerical methods for the solution of problems in conduction of heat. Specifically, an analytical model for the interconnect thermal profile under steady-state condition is proposed in [1] and [2]. The temperature distribution of a global interconnect is governed by the following heat diffusion equations subject to some defined initial values

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} - \frac{1}{\kappa}\frac{\partial T}{\partial t} = -\frac{Q^*}{k_m}, \tag{1}$$

in which κ is the diffusivity of the substance, k_m is the thermal conductivity of the substance, Q^* is the rate of heat generation per unit volume, x, y, z are the space coordinates and t is the time coordinate. It is clear from [3] that the exact solutions available for (1) are practically confined to linear problems on regions of simple shapes. If bodies of complicated shapes, or non-linear boundary conditions, have to be considered, we need to use numerical methods. Some finite differential methods including explicit and implicit methods with truncation error $TR = O[(\triangle t), (\triangle x)^2, (\triangle y)^2, (\triangle z)^2]$ in which O is the order of approximation, and the Crank-Nicolson method with the best accuracy $TR = O[(\triangle t)^2, (\triangle x)^2, (\triangle y)^2, (\triangle z)^2]$ can be found in [3] and [4]. Since these methods are computationally intensive for 2-D or 3-D problems, Peaceman and Rachford [5] and Douglas and Gunn [6] developed the Alternating-Direction-Implicit (ADI) method to overcome this difficulty. Basically, the ADI method is a process to reduce the 2-D or 3-D problems to a succession of two or three one-dimensional problems.

Numerous efforts have been made to perform thermal analysis. The finite difference method with equivalent RC model has been presented in [7], [8]. These methods suffer from superlinear runtime and memory usage for large scale problems due to the complexity of solving large scale matrix equations. Wang and Chen [9], [10] incorporated the finite difference methods with the ADI method and developed a linear-time chip-level dynamic thermal-simulation algorithm based on ADI method, and applied the methods to the thermal simulation of 2-D and 3-D RC models. Because of the obvious unconditionally stable advantage over the explicit methods which are not, implicit and Crank-Nicolson finite difference methods are often used in thermal simulations. However, due to the computational complexity and numerical instability of the inversion of large scale matrices, existing finite difference methods are confined to a best accuracy of second-order accuracy in space and time.

In this paper, we propose an unconditionally stable finite difference methods based on the numerically stable computation of the inverse of large scale matrices proposed by J. Jain *et al.* in [11], with a best accuracy of fourth-order in space and second-order in time. Numerical results of interconnect thermal simulation are presented together with some concluding remarks and future insights.

II. Finite difference formulation of interconnect thermal profile

Fig. 1 shows an interconnect line of length l, width w and thickness h_m and thermal conductivity k_m that passes over the Silicon substrate with an insulator of thickness h_{ins} and an insulator thermal conductivity k_{ins}. Although the thermal conductivity k_m is generally a function of temperature and position, due to its rather small variations in conduction, k_m is often assumed to be constant when analyzing VLSI interconnection lines. In addition, the four sidewalls and the top surface of the chip containing the interconnect lines are presumed to be completely insulated (which is generally a valid assumption) [1]. This means that the interconnect line can only exchange heat with the external environment through

978-1-4244-2342-2/08/$25.00 ©2008 IEEE.

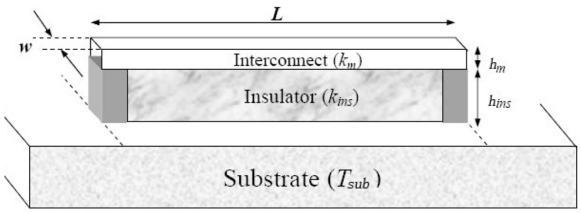

Fig. 1. An interconnect line passing over the substate, separated by an insulation layer.

the two vias at its two ends connected to the substrate. Also, for a global interconnect line whose length is much larger than its width and thickness, a 1-D heat diffusion equation along the length of the interconnect line is often employed. Based on these simplifying assumptions, (1) can be reduced to

$$\frac{\partial^2 T}{\partial x^2} - \frac{1}{\kappa}\frac{\partial T}{\partial t} = -\frac{Q^*}{k_m}, \tag{2}$$

with T a prescribed function of x and t. The effective volumetric heat generation Q^* is defined as the power dissipation minus the heat flow from the interconnect to the substrate per unit volume in [1] and [2], and (2) can be further reduced as

$$\begin{aligned}
&\frac{\partial^2 T}{\partial x^2} - \frac{1}{\kappa}\frac{\partial T}{\partial t} = \lambda_1 T - \lambda_2 T_{chip} - \theta, \text{ in which}\\
&\lambda_1 = \frac{1}{k_m}\left(\frac{k_{ins}}{h_m h_{ins}} - \frac{\rho_i \beta I_{rms}^2}{w^2 h_m^2}\right),\ \lambda_2 = \frac{1}{k_m}\frac{k_{ins}}{h_m h_{ins}},\\
&\text{and } \theta = \frac{1}{k_m}\frac{\rho_i I_{rms}^2}{w^2 h_m^2},
\end{aligned} \tag{3}$$

where ρ_i is the electrical resistivity of the interconnect at the reference temperature and β is the temperature coefficient of resistance.

The finite difference method relies on discretizing a function on a grid. The first step to establish a finite-difference solution method of the partial differential equation (PDE) is to discretize the continuous x coordinate into a finite number of grid points with an interval $(\triangle x)$. At a time step n with time interval $(\triangle t)$, the temperature $T(x,t)$ at point $(i), i = 0, 1, \ldots, N$ can be replaced by $T(i(\triangle x), n(\triangle t))$ which will be denoted by T_i^n in the rest of the paper. The next step is to consider the time discretization problem, three time-marching schemes can be considered to apply on $\frac{\partial T}{\partial t}$ in (2) with respect to accuracy and stability [9], [10]: simple explicit method, simple implicit method and Crank-Nicolson (CN) method. Since CN methods have better truncation error than simple explicit or implicit methods, CN methods will be used in this paper for interconnect thermal simulation.

A. Crank-Nicolson Method with fourth-order spatial accuracy

Crank and Nicolson deal with the time marching by taking the average of simple explicit and implicit methods. They take the difference approximation of $\frac{\partial^2 T}{\partial x^2}$ and $\frac{\partial T}{\partial t}$ at the same time point, and take the average of the central difference approximations of $\frac{\partial^2 T}{\partial x^2}$ at the points n and $n+1$

$$\frac{1}{2}\frac{\partial^2 T}{\partial x^2}\Big|_i^n + \frac{1}{2}\frac{\partial^2 T}{\partial x^2}\Big|_i^{n+1} - \frac{1}{\kappa}\frac{\partial T}{\partial t}\Big|_i^{n+\frac{1}{2}} = -\frac{Q^*}{k_m}. \tag{4}$$

Using approximations

$$\begin{aligned}
\frac{\partial^2 T}{\partial x^2} &= \frac{-T_{i+2} + 16T_{i+1} - 30T_i + 16T_{i-1} - T_{i-2}}{12(\triangle x)^2},\\
\frac{\partial T}{\partial t} &= \frac{T_i^{n+1} - T_i^n}{\triangle t}
\end{aligned}$$

in (4) applicable to both time steps at n and $n+1$ and skipping the right hand side for now to test the stability of the method, yields

$$\begin{aligned}
&rT_{i+2}^{n+1} - 16rT_{i+1}^{n+1} + (30r+1)T_i^{n+1} - 16rT_{i-1}^{n+1} + rT_{i-2}^{n+1} =\\
&-rT_{i+2}^{n} + 16rT_{i+1}^{n} - (30r-1)T_i^{n} + 16rT_{i-1}^{n} - rT_{i-2}^{n}
\end{aligned} \tag{5}$$

where $r = \kappa(\triangle t)/(24(\triangle x)^2)$. Equation (5) does not give the solution of T_i^{n+1} explicitly, which requires the inversion of a symmetric banded matrix with a bandwidth of 5. To find the stability condition of (5), the trial solution

$$T_i^n = \lambda^k e^{j(i\pi/P)},\ j = \sqrt{-1},\ \text{(P is any nonzero integer)}$$

is applied to (5) to get

$$\lambda = \frac{1 - 4r((\cos(\pi/P) - 4)^2 - 9)}{1 + 4r((\cos(\pi/P) - 4)^2 - 9)},\ |\lambda| \le 1, \tag{6}$$

therefore, the CN method is unconditionally stable with best accuracy $TR = O[(\triangle t)^2, (\triangle x)^4]$. The difference equations of (3) have the expression

$$\begin{aligned}
&rT_{i+2}^{n+1} - 16rT_{i+1}^{n+1} + (30r+1)T_i^{n+1} - 16rT_{i-1}^{n+1} + rT_{i-2}^{n+1}\\
&-rT_{i+2}^{n} + 16rT_{i+1}^{n} - (30r-1+R_1)T_i^{n} + 16rT_{i-1}^{n} - rT_{i-2}^{n}\\
&+R_2,
\end{aligned} \tag{7}$$

where $R_1 = \kappa \triangle t\lambda_1$, $R_2 = \kappa \triangle t(\lambda_2 T_{chip} + \theta)$ and $i = 0, 1, \ldots, N$.

B. Boundary conditions

By assumption, the interconnect can only exchange heat with external environment through the its two terminal vias connected to the substrate. Therefore the boundary condition is an adiabatic one

$$\kappa\frac{\partial T(x,t)}{\partial n_i} = 0,$$

where $\frac{\partial}{\partial n_i}$ is the differentiation along the outward direction normal to the boundary surface. Applying the boundary condition to the end points at $i(\triangle x)$, where $i = 0$ and $i = N$, yields

$$-\kappa\frac{\partial T}{\partial x} = 0,\ \text{at } i = 0\ , N \tag{8}$$

From (5), at $i = 0$ two virtual points T_{-1} and T_{-2} are needed and they can be derived by applying (8) as

$$T_{-1} = T_1,\ \text{and } T_{-2} = T_2,. \tag{9}$$

Replacing the virtual points occurring on the boundary points in the difference equations with (9) at $i=0$ and $i=1$, we have the expression

$$\begin{array}{l} rT_2^{n+1}-16rT_1^{n+1}+(15r+0.5)T_0^{n+1}= \\ -rT_2^n+16rT_1^n-(15r-0.5+\frac{R_1}{2})T_0^n+R_2,\ i=0, \\ T_3^{n+1}-16T_2^{n+1}+(31\hat{r}+1)T_1^{n+1}-16rT_0^{n+1}= \\ -rT_3^n+16rT_2^n-(31r-1+R_1)T_1^n+16r)T_0^n+R2,\ i=1. \end{array} \tag{10}$$

Boundary condition expressions at $i=N-1$ and $i=N$ can be similarly achieved.

III. Inversion of Banded matrices

From the discussion in Section II, it can be seen that Crank-Nicolson method requires the inversion of a symmetric band matrix with a bandwidth of 5. In [11], J. Jain *et al.* proposed a numerically stable algorithm, defining D_i and S_i sequences, for the inversion of block-tridiagonal and banded matrices. For a symmetric block-tridiagonal matrix A of the form

$$A=\begin{pmatrix} A_1 & -B_1 & & & \\ -B_1^T & A_2 & -B_2 & & \\ & \ddots & \ddots & \ddots & \\ & & -B_{N_y-2}^T & A_{N_y-1} & -B_{N_y-1} \\ & & & -B_{N_y-1}^T & A_{N_y} \end{pmatrix}, \tag{11}$$

where each $A_i, B_i \in C^{N_x\times N_y}$, thus $A\in C^{N_yN_x\times N_yN_x}$ with N_y diagonal blocks of size N_x each. S_i sequence can be computed in $O(N_yN_x^3)$ operations using the following numerically stable recursion:

$$\begin{array}{l} S_{N_y-1}=B_{N_y-1}A_{N_y}^{-1}, \\ S_i=B_i(A_{i+1}-S_{i+1}B_{i+1}^T)^{-1},\ i=N_y-2,\ldots,1. \end{array} \tag{12}$$

It is readily verified that the diagonal blocks of A^{-1}, denoted sequence D_i, are given by the recursion

$$\begin{array}{l} D_1=(A_1-B_1S_1^T)^{-1}, \\ D_{N_y}=A_{N_y}^{-1}(I+B_{N_y-1}^TD_{N_y-1}S_{N_y-1}), \\ D_i=(A_i-B_iS_i^T)^{-1}(I+B_{i-1}^TD_{i-1}S_{i-1}), \\ i=2,\ldots,N_y-1, \end{array} \tag{13}$$

while the remaining block entries can be computed in a numerically stable way as

$$A_{ij}^{-1}=D_iS_iS_{i+1}\ldots S_{j-1},\ j>i, \tag{14}$$

since A^{-1} is symmetric, combining (13) and (14), A^{-1} is computed. A fast computation of the product of the inverse of a block-tridiagonal matrix A and a vector x is also proposed in [11] with a computation time of $O(N_yN_x^2)$ as compared to $O(N_y^2N_x^2)$ otherwise.

The symmetric banded matrix to be inverted with bandwidth 5 can be considered as a block-tridiagonal matrix by grouping into blocks of size 2×2, to be in the same structure as A in (11), with

$$A_i=\begin{pmatrix} 30r+1 & -16r \\ -16r & 30r+1 \end{pmatrix}\ B_i=\begin{pmatrix} -r & 0 \\ 16r & -r \end{pmatrix}. \tag{15}$$

Incorporating the boundary condition expressions into the set of equations, the symmetric banded matrix to be inverted has the structure in (11) with the off-diagonal matrices B_i in (14) and the first diagonal block matrix A_1, last diagonal block matrix A_{Ny}

$$A_1=\begin{pmatrix} 15r+0.5 & -16r \\ -16r & 31r+1 \end{pmatrix},$$
$$A_{Ny}=\begin{pmatrix} 31r+1 & -16r \\ -16r & 15r+0.5 \end{pmatrix},$$

and the remaining diagonal matrices A_i in (14).

In this paper, we use this numerically stable method for inversion of block-tridiagonal and banded matrices and the fast algorithm of computing $A^{-1}x$ in [11] to compute (7) together with boundary conditions (10). Consequently, the proposed finite difference method has fourth-order accuracy in space and second-order accuracy in time.

IV. Experimental Results

In this section, simulation results of interconnect thermal profile described by (3) will be presented. Equation (3) shows that the underlying substrate temperature, T_{chip}, plays an important role in determining the temperature of the line T. This value is usually assumed to be constant through the substrate surface. Due to the very small thermal resistivity of the vias, the temperature at the two sides of the metal line is equal to that of the substrate. Therefore, the initial conditions to solve (7) together with boundary conditions (10) can be defined as

$$T|_{i=1}=T_{chip},\ \text{and}\ T|_{i=I}=T_{chip}. \tag{16}$$

Assuming a uniform substrate temperature of $T_{chip}=100^oC$, the steady state of interconnect thermal profiles for global lines using CN with 2nd and 4th order spatial accuracy are presented in Fig. 2 and Fig. 3. From the figures, the proposed CN method and the traditional CN method both converge to the steady state. However, temperature profiles before reaching the steady state are different. Temperature difference between the two CN methods at iteration 10 is shown in Fig. 4. It can be seen in Fig. 2 and Fig. 3 that interconnect temperature can reach as high as 140^oC. Such a temperature can significantly increase the interconnect resistance, which in turn would increase the signal propagation delay in the interconnect line. In Fig. 4, before the two CN methods converge to the steady state, we observe temperature difference in the temperature profiles. Since the proposed CN method is of higher order spatial accuracy, it will present a more accurate temperature profile than the traditional CN method.

The computation time of the inversion of the banded matrix is $O(N_yN_x^3)$, and the computation time of the fast algorithm of $A^{-1}x$ is $O(N_yN_x^2)$. In the proposed method, $Nx=2$ which is very small and $NxNy=N$, thus the overall computation time of the proposed method will be $O(N)$, which means the run time of the proposed method

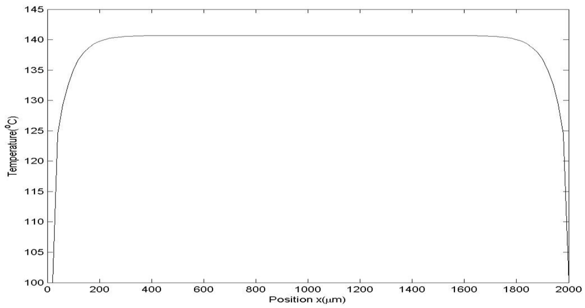

Fig. 2. Thermal profile along the length of a $2000\mu m$ long interconnect line with a uniform substrate temperature using CN with 4th-order spatial accuracy.

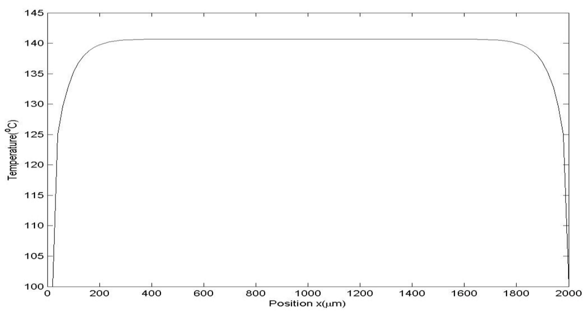

Fig. 3. Thermal profile along the length of a $2000\mu m$ long interconnect line with a uniform substrate temperature using CN with 2nd-order spatial accuracy.

is linearly proportional to the number of nodes. It should also be noted that the uniform substrate temperature profile is a valid assumption for local short interconnects, but is not true in the case of global long lines in the upper metal layers. Therefore, to achieve an accurate interconnect thermal profile, non-uniform substrate temperature profile has to be considered.

The unconditional stability of the proposed CN method and the traditional CN method guarantee their convergence to the exact steady thermal state. Consequently, with the number of iteration increasing, the temperature difference between the two methods will decrease and will eventually vanish when the steady state is reached. Because of the higher spatial accuracy of the proposed CN method, although it does not provide a more accurate final and steady temperature profile than the traditional CN method, it does provide a more accurate one before the steady temperature state is reached, especially at the early stages of the simulation.

V. CONCLUSIONS

We have presented in this paper a finite difference method to simulate interconnect temperature profile with improved spatial accuracy. Crank-Nicolson method with accuracy $TR = O[(\triangle x)^4, (\triangle t)^2]$ has been described, its accuracy

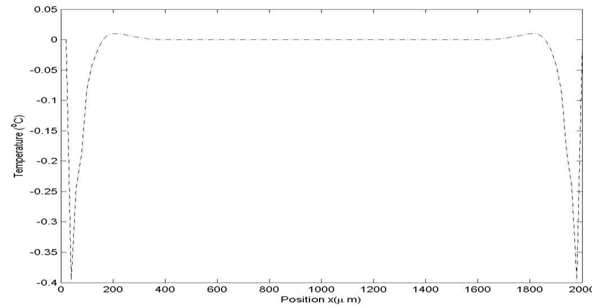

Fig. 4. Temperature difference of the proposed CN method with 4th-order spatial accuracy and the traditional CN method with 2nd-order spatial accuracy at iteration 10.

and stability condition discussed. Thermal simulation of a global interconnect is conducted using the proposed method. The simulation results show that under a uniform substrate temperature profile, the proposed CN method can have a better thermal profile than the traditional CN method with $TR = O[(\triangle x)^2, (\triangle t)^2]$ before reaching the steady state. The runtime of the proposed Crank-Nicolson method is linearly proportional to the number of nodes. This method can also be applied to two- or three-dimensional problems using the ADI method.

REFERENCES

[1] A. H. Ajami, K. Banerjee, and M. Pedram, "Modeling and analysis of non-uniform substrate temperature effects in high performance vlsi," *IEEE Trans. on Computer Aided Design*, vol. 24, no. 6, pp. 849–861, 2005.

[2] M. Pedram and S. Nazarian, "Thermal modeling, analysis and management in vlsi circuits: principles and methods," *Proc. of IEEE, Special Issue on Thermal Analysis of ULSI*, vol. 94, no. 8, pp. 1487–1501, 2006.

[3] H. S. Carslaw and J. C. Jaeger, *Conduction of heat in solids*. London: Oxford University Press, 1948.

[4] M. N. Ozisik, *Finite difference*. New York: CRC, 1994.

[5] D. W. Peaceman and J. H. H. Rachford, "The numerical solution of parabolic and elliptic defferential equations," *J. Soc. Ind. Appl. Math.*, vol. 3, pp. 28–41, 1955.

[6] J. J. Douglas and J. E. Gunn, "A general formulation of alternating direction methods-part I: Parabolic and hyperbolic problems," *Numer. Math.*, vol. 6, pp. 428–453, 1964.

[7] Y. K. Cheng, P. Raha., C. C. Teng, E. Rosenbaum, and S. M. Kang, "Illiads-t: An telectrothermal timing simulator for temperature-sensitive reliability diagnosis of comos vlsi chips," *IEEE Tans. Computer-Aided Design*, vol. 17, pp. 668–681, 1998.

[8] D. Chen, E. Li, E. Rosenbaum, and S. M. Kang, "Interconnect thermal modeling for accurate simluation of ciurcuit timing and reliability," *IEEE Tans. Computer-Aided Design*, vol. 19, pp. 197–205, 2000.

[9] T.-Y. Wang and C. C.-P. Chen, "3-D Thermal-ADI: a linear-time chip level transient thermal simulator," *IEEE Transactions on Computer-Aided Design of Integrated Circuits And Systems (TCAD)*, vol. 21, no. 11, pp. 1343 –1352, 2002.

[10] ——, "Thermal-ADI: A linear-time chip-level dynamic thermal simulation algorithm based on alternating-direction-implicit (ADI) method," *IEEE Transaction on Very Large Scale Integration Systems (TVLSI)*, vol. 11, no. 4, pp. 691– 700, 2003.

[11] J. Jain, S. Cauley, H. Li, C. Koh, and V. Balakrishnan, "Numerically stable algorithms for inversion of block tridiagonal and banded matrices," Electrical and Computer Engineering, Purdue University, West Lafayette, Tech. Rep. IN 47907-1285, 2006.