Transient Thermal Analysis of 3-D Integrated Circuits Packages by the DGTD Method

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***Abstract*— Since accurate thermal analysis plays a critical role in the thermal design and management of the 3-D system-level integration, in this paper, a discontinuous Galerkin time-domain (DGTD) algorithm is proposed to achieve this purpose. Such as the parabolic partial differential equation (PDE), the transient thermal equation cannot be directly solved by the DGTD method. To address this issue, the heat flux, as an auxiliary variable, is introduced to reduce the Laplace operator to a divergence operator. The resulting PDE is hyperbolic, which can be further written into a conservative form. By properly choosing the definition of the numerical flux used for the information exchange between neighboring elements, the hyperbolic thermal PDE can be solved by the DGTD together with the auxiliary differential equation. The proposed algorithm is a kind of element-level domain decomposition method, which is suitable to deal with multiscale geometries in 3-D integrated systems. To verify the accuracy and robustness of the developed DGTD algorithm, several representative examples are benchmarked.**

***Index Terms*— Auxiliary-differential equation (ADE) method, discontinuous Galerkin time-domain (DGTD) method, integrated circuit package, numerical flux, transient thermal analysis.**

I. Introduction

FOLLOWING the Moore's law, the number of transistors in a single chip has raised from a few thousands in 1970s to several billions in 2010s, while the electrical size has been continuously downscaling. Further fueled by the advanced 3-D packaging technologies such as system on package [1], [2] and interconnection technologies like the through silicon-vias (TSV) [3], heterogeneous modules and chips are capable of being vertically stacked up together by TSVs and redistribution traces, which thus makes the possibility to integrate multiple different functional modules into a limited space. On the other hand, it simultaneously brings significant challenges in the thermal management. Improper thermal designs would not only degrade the system performance, but also lead to serious reliability issues. Therefore, accurate and robust thermal analysis is essential at the design stage.

To achieve this purpose, numerous modalities have been proposed in the past decades to characterize the thermal properties of the integrated circuits, for instance, the analytical approaches [4] and numerical algorithms such as the finite element method (FEM) [5], [6] and finite difference method (FDM) [7]–[9]. The analytical method in [4] proposed an equivalent thermal circuit model to describe the temperature variation, which is convenient and efficient to provide a guideline at the design stage although it is not comprehensive and exactly rigorous. Recently, researchers proposed a noniterative heat transfer model [10], [11] to predict the steady-state temperature distributions in 3-D chips, the accuracy of the analytical method is comparable to FEM. On the other hand, the numerical methods are rigorous but less efficient. In [5] and [6], to handle the multiscale properties of the 3-D integrated circuit packages, a domain decomposition method (DDM)-based FEM was proposed, which converges significantly fast while conventional FEM would fail to converge. In [12]–[14], the efficiency of the FEM is further improved by the parallel computing techniques. Thus, more complicated structures can be modeled within less computational cost. Besides the FEM, in [7] and [8], the FDM was employed to facilitate the thermal analysis. Specifically, an equivalent circuit network was derived based on the FDM formulated equations in [9] that builds up the relation between thermal models and equivalent circuit networks. In [15] and [16], an FDM-based thermal solver named "HotSpot," which is based on the equivalent circuit of thermal resistance and capacitances of microarchitecture blocks, is widely applied to analyze thermal distributions of integration circuits. Compared to the FEM, the FDM is more convenient and simple to implement, but lacks the flexibility to address irregular geometries.

In this paper, a discontinuous Galerkin time-domain (DGTD) method [17]–[20] is proposed to conduct the transient thermal analysis for complicated integrated circuits packages. Compared to the finite-difference time-domain method, the

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DGTD method is capable of modeling arbitrary shapes and simultaneously can achieve high-order accuracy by adopting hierarchical basis functions. Similar to the finite volume method [21], all operators in the DGTD analysis are local, and the information exchange between the neighboring mesh elements is implemented by a term called numerical flux. Therefore, unlike FEM, the matrix equations are locally established with dimension equal to the number of degrees of freedom in the corresponding mesh element. Thus, the formulated mass-matrices are block-diagonal and can be directly inverted with negligible computational cost. Since the solutions across the interfaces of adjacent elements are allowed to be discontinuous, the DGTD method owns more flexibilities to choose the type and the order of basis functions in each element [22]. In fact, the DGTD method can be considered as an element-level DDM. Therefore, the DGTD method is more preferable for large and/or multiscale geometries in which a large number of heterogeneous meshes are involved [23]. If the conventional FEM was used, the ill-conditioned matrix equations resulted from inhomogeneous mesh elements would converge very slowly or even not converge at all. Alternatively, the complicated domain decomposition FEM has to be resorted [5], [6].

Since the DGTD method is amenable to the hyperbolic systems, the thermal equation as a parabolic partial differential equation (PDE) is thus unable to be solved by the DGTD algorithm directly [17]. To handle this problem, an auxiliary variable named heat flux is introduced with the aim to degenerate the high-order spatial differential operator (Laplace operator ∇^2) to a first-order operator (divergence operator $\nabla\cdot$). Then, the thermal equation is transformed to be a hyperbolic PDE that can be written into a conservative form. Together with the differential equation governing the auxiliary variable, the newly constructed thermal equation can be solved by the DGTD method. To validate the feasibility, the accuracy, and the robustness of the developed DGTD method, several representative examples including the 3-D integration with complex structures are given.

The remainder of this paper is organized as follows. In Section II, the theory and mathematical details about the degeneration of the parabolic equation to a hyperbolic one and the formulation matrix equations by the DGTD method are described. In Section III, numerical examples are presented to validate the proposed algorithm. Conclusions and discussions are given at the end of this paper.

II. Theory and Mathematical Formulation

Suppose that the domain of interest for the thermal analysis is denoted as $\boldsymbol{\Omega}$ and simultaneously bounded by the boundary $\partial\boldsymbol{\Omega}$, its temporal temperature variation in this thermal system is governed by a first-order time-derivative PDE defined as [5], [12]

$$\nabla \cdot \kappa \nabla T + Q = \rho_m c_\rho \frac{\partial T}{\partial t} \tag{1}$$

where T denotes the temperature distribution, κ represents the thermal conductivity, Q is the heat source, and ρ_m and c_ρ are the mass density of the material and specific heat capacity, respectively. To solve (1), we have the Dirichlet boundary condition at the boundary $\partial\boldsymbol{\Omega}$

$$T = T_{\partial\Omega} \tag{2}$$

and the convection boundary condition

$$\hat{\mathbf{n}} \cdot \kappa \nabla T = -h(T - T_a) \tag{3}$$

or

$$\kappa \frac{\partial T}{\partial n} = -h(T - T_a) \tag{4}$$

with $\hat{\mathbf{n}}$ representing the unit outward normal vector perpendicular to the boundary surface, and h and T_a denoting the convective heat transfer coefficient and the ambient temperature, respectively.

Since the PDE in (1) is a parabolic differential equation, the DGTD algorithm cannot be straightforwardly applied to solve it. Instead, (1) has to be transformed to a hyperbolic equation that is able to be written into a conservative form. Motivated by this aim, an intermediate vector variable $\mathbf{q}(x, y, z, t)$ is introduced, which is given by

$$\mathbf{q}(x, y, z, t) = -\kappa \nabla T. \tag{5}$$

The auxiliary variable $\mathbf{q}$ actually denotes the heat flux or the rate of heat transfer through a surface per unit time.

With the auxiliary equation (5), the second-order spatial-derivation (the Laplace operator) in (1) can be decreased to a first-order divergence operator. Consequently, (1) can be rewritten as

$$-\nabla \cdot \mathbf{q} + Q = \rho_m c_\rho \frac{\partial T}{\partial t} \tag{6}$$

which is now in a form of conservation.

In this paper, the main focus is to validate the feasibility of DGTD method in solving the transient thermal equation, where the thermal conductivity and the specific heat capacity in (5) and (6) are assumed to be temperature independent. The temperature-dependent situation will be investigated in the future DGTD-based electrical-thermal cosimulation solver, in which the electrical conductivity is also considered to be temperature dependent.

To solve (5) and (6) by the DGTD method, the computational domain $\boldsymbol{\Omega}$ is first split into a number of nonoverlapping polyhedron elements $\boldsymbol{\Omega}_i$ (In this paper, tetrahedrons are used to flexibly model the irregular geometries). In each element i, the nodal basis functions $\psi(\mathbf{r})$, $\phi(\mathbf{r})$, $\varphi(\mathbf{r})$, and $\gamma(\mathbf{r})$ are employed to approximate T, q_x, q_y, and q_z, respectively. By implementing the DG testing over (5) and each component of (6), we have

$$\rho_m c_\rho \int_{\Omega_i} \psi_k^i \frac{\partial T^i}{\partial t} dV = \int_{\Omega_i} \psi_k^i \left(-\nabla \cdot \mathbf{q}^i + Q^i\right) dV \tag{7}$$

$$\int_{\Omega_i} \phi_k^i q_x^i dV = -\kappa \int_{\Omega_i} \phi_k^i \cdot \nabla_x T^i dV \tag{8}$$

$$\int_{\Omega_i} \varphi_k^i q_y^i dV = -\kappa \int_{\Omega_i} \varphi_k^i \cdot \nabla_y T^i dV \tag{9}$$

$$\int_{\Omega_i} \gamma_k^i q_z^i dV = -\kappa \int_{\Omega_i} \gamma_k^i \cdot \nabla_z T^i dV \tag{10}$$

with $\nabla_x T = \partial_x T$, $\nabla_y T = \partial_y T$, and $\nabla_z T = \partial_z T$.

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Based on the integration by parts and the Gaussian theorem, we have weak formulations of (7)–(10) defined as

$$\rho_m c_\rho \int_{\Omega_i} \psi_k^i \frac{\partial T^i}{\partial t} dV = \int_{\Omega_i} \left(\mathbf{q}^i \cdot \nabla \psi_k^i + \psi_k^i Q^i\right) dV - \sum_{f=1}^{4} \int_{\partial\Omega_i^f} \psi_k^i \hat{\mathbf{n}}_f^i \cdot \mathbf{q}_f^* dS \quad (11)$$

$$\int_{\Omega_i} \phi_k^i \mathbf{q}_x^i dV = \kappa \int_{\Omega_i} T^i \nabla_x \phi_k^i dV - \kappa \sum_{f=1}^{4} \int_{\partial\Omega_i^f} n_{x,f}^i T_f^* \phi_k^i dS \quad (12)$$

$$\int_{\Omega_i} \varphi_k^i \mathbf{q}_y^i dV = \kappa \int_{\Omega_i} T^i \nabla_y \varphi_k^i dV - \kappa \sum_{f=1}^{4} \int_{\partial\Omega_i^f} n_{y,f}^i T_f^* \varphi_k^i dS \quad (13)$$

$$\int_{\Omega_i} \gamma_k^i \mathbf{q}_z^i dV = \kappa \int_{\Omega_i} T^i \nabla_z \gamma_k^i dV - \kappa \sum_{f=1}^{4} \int_{\partial\Omega_i^f} n_{z,f}^i T_f^* \gamma_k^i dS. \quad (14)$$

It is necessary to mention that the solutions in the adjacent elements are allowed to be discontinuous in the DGTD analysis, thus the values of solutions at the interfaces T^*, q_x^*, q_y^*, and q_z^* involved in the surface integration at the right hand sides of (11)–(14) must be carefully chosen in order to obtain an accurate and unique solution. For hyperbolic systems, the numerical fluxes denoted by $\mathbf{q}^*$ and T^* are employed to facilitate the information communication between the neighboring elements. In this paper, we have the following definitions [24]–[26]:

$$\hat{\mathbf{n}}_f^i \cdot \mathbf{q}_f^* = C_{10}\left(\hat{\mathbf{n}}_f^i \cdot \mathbf{q}^i + \hat{\mathbf{n}}_f^i \cdot \mathbf{q}_f^j\right) + C_{11}(\hat{\mathbf{n}}_f^i \cdot \mathbf{q}^i - \hat{\mathbf{n}}_f^i \cdot \mathbf{q}_f^j) + C_{12}(T^i - T_f^j) \quad (15)$$

$$T_f^* = C_{20}(T^i + T_f^j) + C_{21}(\hat{\mathbf{n}}_f^i \cdot \mathbf{q}^i - \hat{\mathbf{n}}_f^i \cdot \mathbf{q}^j) + C_{22}(T^i - T_f^j) \quad (16)$$

where the superscript j denotes the neighboring element, $\mathbf{n}_f^i$ represents the unit normal vector at face f, and the coefficients $C_{10} = 0.5$, $C_{11} = 0$, $C_{12} = -4$, $C_{20} = 0.5$, $C_{21} = 0$, and $C_{22} = 0$. Specifically, to consider the convection boundary condition in (3) and (4), C_{10}, C_{12}, and C_{22} are redefined as 0, $-h$, and 0.5, respectively.

Next, the unknowns in element i are approximated by the local nodal basis functions: $T^i = \sum_{k=1}^{n_T} \psi_k^i(\mathbf{r})\tilde{T}_k^i(t)$, $q_x^i = \sum_{k=1}^{n_q^i} \phi_k^i(\mathbf{r})\tilde{q}_x^i(t)$, $q_y^i = \sum_{k=1}^{n_q^i} \varphi_k^i(\mathbf{r})\tilde{q}_y^i(t)$, and $q_z = \sum_{k=1}^{n_q^i} \gamma(\mathbf{r})\tilde{q}_z^i(t)$ with n_T^i and n_q^i denoting the number of basis functions for T^i and $q_{x,y,z}^i$, while $\tilde{T}_k^i(t)$, $\tilde{q}_x^i(t)$, $\tilde{q}_y^i(t)$, and $\tilde{q}_z^i(t)$ represent the time-dependent expansion coefficients that are to be determined. By further resorting to (11)–(14) and the definitions of numerical fluxes in (15) and (16), four semidiscrete matrix equations can be derived. Namely

$$[\bar{\mathbf{M}}_T^i]\frac{\partial \tilde{\mathbf{T}}^i}{\partial t} = [\bar{\mathbf{S}}_x^i]\tilde{\mathbf{q}}_x^i + [\bar{\mathbf{S}}_y^i]\tilde{\mathbf{q}}_y^i + [\bar{\mathbf{S}}_z^i]\tilde{\mathbf{q}}_z^i + \mathbf{Q}^i + \sum_{f=1}^{4}\Big([\mathbf{F}_{q_x}^{ii}]\tilde{\mathbf{q}}_x^i + [\bar{\mathbf{F}}_{q_y}^{ii}]\tilde{\mathbf{q}}_y^i + [\bar{\mathbf{F}}_{q_z}^{ii}]\tilde{\mathbf{q}}_z^{ii} + [\bar{\mathbf{F}}_{q_x}^{ij}]\tilde{\mathbf{q}}_x^j + [\mathbf{F}_{q_y}^{ij}]\tilde{\mathbf{q}}_y^j + [\bar{\mathbf{F}}_{q_z}^{ij}]\tilde{\mathbf{q}}_z^j + [\bar{\mathbf{F}}_T^{ii}]\tilde{\mathbf{T}}^i + [\mathbf{F}_T^{ij}]\tilde{\mathbf{T}}^j\Big) \quad (17)$$

$$[\bar{\mathbf{M}}_{q_x}^i]\tilde{\mathbf{q}}_x^i = [\bar{\mathbf{C}}_x^i]\tilde{\mathbf{T}}^i + \sum_{f=1}^{4}\left([\bar{\mathbf{G}}_x^{ii}]\tilde{\mathbf{T}}^i + [\mathbf{G}_x^{ij}]\tilde{\mathbf{T}}^j\right) \quad (18)$$

$$[\bar{\mathbf{M}}_{q_y}^i]\tilde{\mathbf{q}}_y^i = [\bar{\mathbf{C}}_y^i]\tilde{\mathbf{T}}^i + \sum_{f=1}^{4}\left([\bar{\mathbf{G}}_y^{ii}]\tilde{\mathbf{T}}^i + [\mathbf{G}_y^{ij}]\tilde{\mathbf{T}}^j\right) \quad (19)$$

$$[\bar{\mathbf{M}}_{q_z}^i]\tilde{\mathbf{q}}_z^i = [\bar{\mathbf{C}}_z^i]\tilde{\mathbf{T}}^i + \sum_{f=1}^{4}\left([\bar{\mathbf{G}}_z^{ii}]\tilde{\mathbf{T}}^i + [\mathbf{G}_z^{ij}]\tilde{\mathbf{T}}^j\right) \quad (20)$$

where the elements in above matrices are given as

$$\begin{aligned}
[\bar{\mathbf{M}}_T^i]_{kl} &= \rho_m c_\rho \int_{\Omega_i} \psi_k^i(\mathbf{r})\psi_l^i(\mathbf{r})dV \\
[\bar{\mathbf{M}}_{q_x}^i]_{kl} &= \int_{\Omega_i} \phi_k^i(\mathbf{r})\phi_l^i(\mathbf{r})dV \\
[\bar{\mathbf{S}}_x^i]_{kl} &= \int_{\Omega_i} \phi_l^i(\mathbf{r})\nabla\psi_k^i(\mathbf{r})dV \\
[\bar{\mathbf{Q}}^i]_k &= \int_{\Omega_i} \phi_k^i(\mathbf{r})QdV \\
[\bar{\mathbf{C}}_x^i]_{kl} &= \kappa \int_{\Omega_i} \psi_l^i(\mathbf{r})\nabla_x\phi_k^i(\mathbf{r})dV \\
[\bar{\mathbf{F}}_{qx}^{ii}]_{kl} &= C_{10}\int_{\partial\Omega_{i,f}} \psi_k^i(\mathbf{r})n_{x,f}^i\phi_l^i(\mathbf{r})dS \\
[\bar{\mathbf{F}}_{qx}^{ij}]_{kl} &= C_{10}\int_{\partial\Omega_{i,f}} \psi_k^i(\mathbf{r})n_{x,f}^i\phi_l^j(\mathbf{r})dS \\
[\bar{\mathbf{F}}_T^{ii}]_{kl} &= C_{12}\int_{\partial\Omega_{i,f}} \psi_k^i(\mathbf{r})\psi_l^i(\mathbf{r})dS \\
[\bar{\mathbf{F}}_T^{ij}]_{kl} &= -C_{12}\int_{\partial\Omega_{i,f}} \psi_k^i(\mathbf{r})\psi_l^j(\mathbf{r})dS \\
[\bar{\mathbf{G}}_x^{ii}]_{kl} &= \kappa(C_{20}+C_{22})\int_{\partial\Omega_{i,f}} \phi_k^i(\mathbf{r})n_{x,f}^i\psi_l^i(\mathbf{r})dS \\
[\bar{\mathbf{G}}_x^{ij}]_{kl} &= \kappa(C_{20}-C_{22})\int_{\partial\Omega_{i,f}} \phi_k^i(\mathbf{r})n_{x,f}^i\psi_l^j(\mathbf{r})dS.
\end{aligned} \quad (21)$$

For other elements in $[\bar{\mathbf{S}}_y^i]$, $[\bar{\mathbf{S}}_z^i]$, $[\bar{\mathbf{C}}_y^i]$, $[\bar{\mathbf{C}}_z^i]$, $[\bar{\mathbf{F}}_{qy}^{ii}]$, $[\bar{\mathbf{F}}_{qz}^{ii}]$, $[\bar{\mathbf{G}}_y^{ii}]$, $[\bar{\mathbf{G}}_z^{ii}]$, $[\bar{\mathbf{G}}_y^{ij}]$, and $[\bar{\mathbf{G}}_z^{ij}]$, their definitions have similar expressions to those in the x-direction.

In this paper, each unknown in every tetrahedron is approximated by four nodal basis functions, namely, $n_T^i = 4$ and $n_q^i = 4$. Therefore, the dimension of the matrix equation to be solved is 4 by 4. As a result, the computational cost for the matrix factorization is negligible.

To keep an explicit time marching scheme, the first-order time-derivative in (17) is discretized by the forward Euler method. For the explicit scheme, the Courant–Friedrichs–Lewy condition must be satisfied to ensure stability. In this

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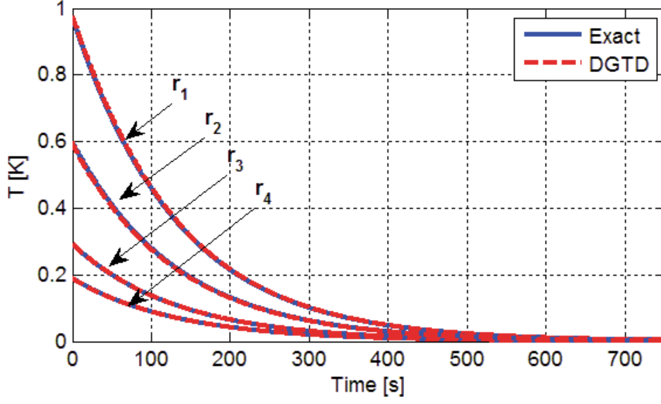


Fig. 1. Calculated temperature T by DGTD at $\mathbf{r}_1 = 0.252\hat{\mathbf{x}}+0.249\hat{\mathbf{y}}+0.284\hat{\mathbf{z}}$, $\mathbf{r}_2 = 0.255\hat{\mathbf{x}} + 0.231\hat{\mathbf{y}} + 0.103\hat{\mathbf{z}}$, $\mathbf{r}_3 = 0.232\hat{\mathbf{x}} + 0.255\hat{\mathbf{y}} + 0.048\hat{\mathbf{z}}$, and $\mathbf{r}_4 = 0.04\hat{\mathbf{x}} + 0.255\hat{\mathbf{y}} + 0.141\hat{\mathbf{z}}$. For comparison, the analytical results (blue curve) obtained from (23) are given as well.

paper, the time-stepping size for the ith element is determined in terms of the following condition:

$$\Delta t \leq \alpha \cdot \min \left\{ l_{\min}^2 / [\kappa/\rho c_\rho] \right\} \tag{22}$$

with α depending on the order of basis function and the type of spatial discretization.

III. Numerical Results

In this section, several representative examples are provided to verify and validate the accuracy of the proposed algorithm.

A. Rectangular Silicon Brick

In order to validate the feasibility and accuracy of the DGTD algorithm subjected to different boundary conditions, a rectangular silicon brick is studied. The dimensions of the brick in the x-, y-, and z-directions are given by $L_x = 0.5$ m, $L_y = 0.5$ m, and $L_z = 0.5$ m, respectively. First, the DGTD algorithm is benchmarked with the Dirichlet boundary condition: $T(x, y, z, t)|_{x=0} = 0$, $T(x, y, z, t)|_{x=L_x} = 0$, $T(x, y, z, t)|_{z=0} = 0$, $T(x, y, z, t)|_{z=L_z} = 0$, and the initial solution $T(x, y, z, t)|_{t=0} = \sin(\pi x/L_x)\sin(\pi z/L_z)$. Correspondingly, we have the analytical solution described as

$$T(x, y, z, t) = \sin\left(\frac{\pi x}{L_x}\right) \sin\left(\frac{\pi z}{L_z}\right) \times \exp\left[-\frac{\kappa \pi^2 t}{\rho c_\rho}\left(\frac{1}{L_x^2} + \frac{1}{L_z^2}\right)\right] \tag{23}$$

with $\kappa = 160$ W/[m.K], $\rho = 2300$ kg/m^3,and $c_\rho = 730$ J/[kg.K] in this simulation.

After the DGTD analysis, the computed temperature profiles at four different points are plotted versus the time as shown in Fig. 1. It is noted that the numerical results are in good consistence with the analytical references. In Fig. 2, the 3-D temperature distribution at $t = 12.4$ s is also given. For comparison, the analytical reference is provided again. Very good agreement between the numerical results and the reference solutions is observed. To have a better clarification, the L_2 norm errors at the four observation points are calculated as 8.41×10^{-3}, 9.78×10^{-3}, 2.14×10^{-3}, and 3.22×10^{-3}. Thus, the accuracy of DGTD for the Dirichlet boundary condition is successfully demonstrated. In the DGTD method, the implementation of Dirichlet boundary condition is similar to that in the FEM, for nodes at the Dirichlet boundary, the unknown coefficients of the corresponding nodal basis are explicitly given. Thus, only unknowns not over the Dirichlet boundary condition are to be solved.

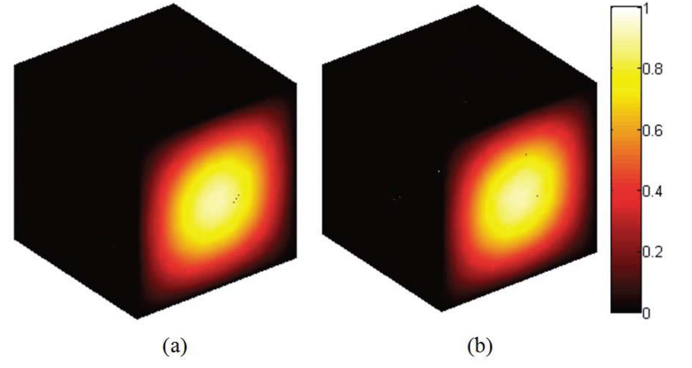
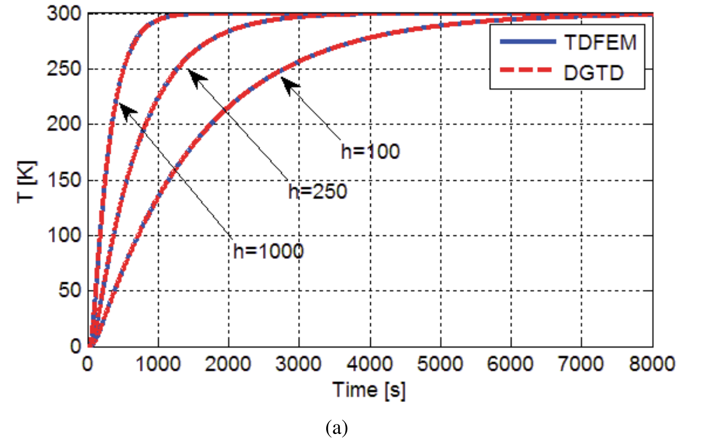
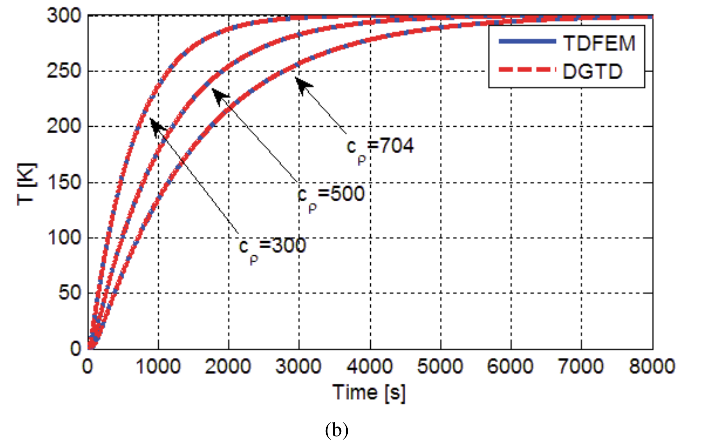


Fig. 2. 3-D transient temperature (K) obtained by (a) DGTD simulation and (b) analytical formula (23).



(a)



(b)

Fig. 3. Calculated temporal temperature at $\mathbf{r} = 0.185\hat{\mathbf{x}} + 0.18\hat{\mathbf{y}} + 0.256\hat{\mathbf{z}}$ for (a) different convective heat transfer coefficients and (b) specific heat capacity. For comparison, the results from the TDFEM are given as well.

In practical thermal systems, the convective boundary condition must be considered since air cooling is popularly

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TABLE I
GEOMETRY INFORMATION AND EQUIVALENT THERMAL PARAMETERS

Layer	Dimension (mm^3)	Material	κ (W/[m·K])	ρ (kg/m^3)	c_ρ (J/[kg.K])
TIM	$10 \times 10 \times 0.75$	epoxy	1.6	3100	610
Die	$10 \times 10 \times 1.25$	Si	130	2329	700
Microbump-1	$10 \times 10 \times 0.25$	SnAg & epoxy	⊥0.9, //0.6	1547	1381
Interposer	$30 \times 30 \times 0.5$	Cu & Si	⊥170, //25	3197	583
Microbump-2	$30 \times 30 \times 0.75$	SnAg & epoxy	⊥0.9, //0.6	1547	1381
Package	$48 \times 48 \times 4.5$	FR4	0.3	1900	1369

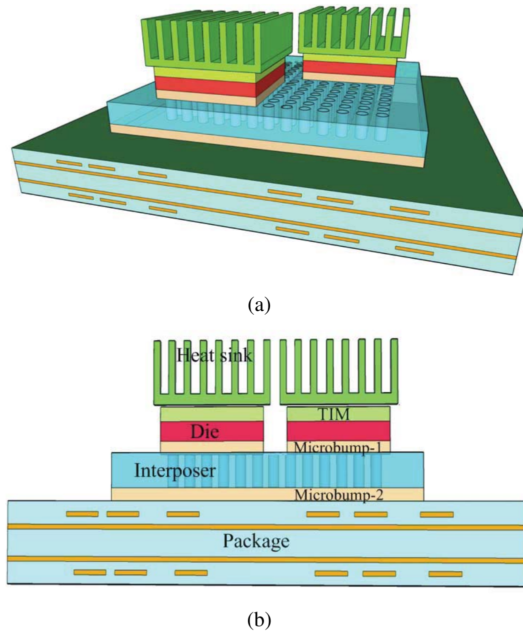

Fig. 4. (a) 3-D view of the integrated system. (b) Cross-sectional view of the structure.

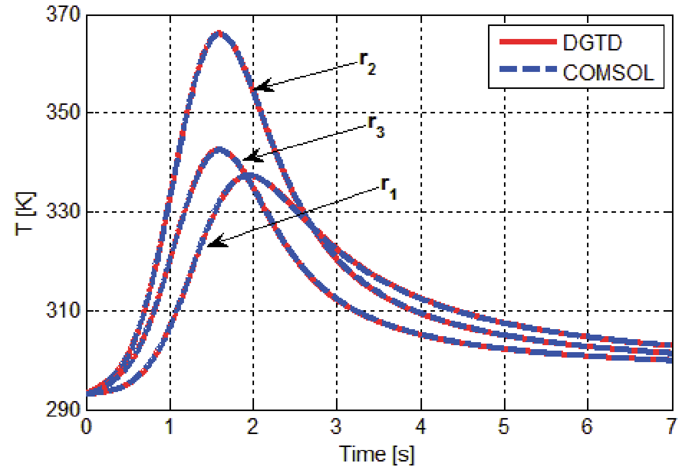

Fig. 5. DGTD calculated temperature at three observation points $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_3$. For verification purposes, the results simulated by COMSOL are also given.

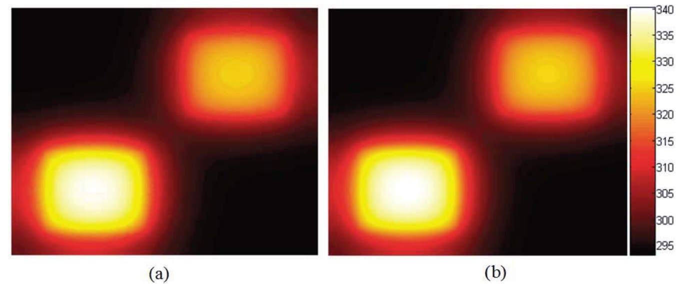

Fig. 6. Snapshot of the temperature profile (K) at the top surface of the interposer at $t = 2$ s. (a) Numerical result by the DGTD method. (b) Reference by COMSOL.

employed to cool down the integrated chips. To achieve this purpose, the six boundary surfaces of the above brick are imposed with the convective boundary.

We first suppose that the parameters including the thermal conductivity κ, the mass density ρ, the specific heat capacity c_ρ, and the ambient temperature T_a are fixed to 135 $\mathrm{W/[m \cdot K]}$, 2330 $\mathrm{kg/m^3}$, 704 $\mathrm{J/[kg \cdot K]}$, and 300 K, respectively, while the convective heat transfer coefficient h is set to be different values. In Fig. 3(a), the temporal temperature at $\mathbf{r} = 0.185\hat{\mathbf{x}}+0.18\hat{\mathbf{y}}+0.256\hat{\mathbf{z}}$ is provided. As can be seen, the temperature increases faster for larger convection coefficient. For comparison, the results from the time domain FEM (TDFEM) are given. As can be seen, obvious consistencies are reached. The L_2 norm errors corresponding to $h = 100$, 250, and 1000 are 1.56×10^{-4}, 2.75×10^{-4}, and 5.84×10^{-4}, respectively.

Next, the convective heat transfer coefficient h is fixed to be 100 $\mathrm{W/[m^2 \cdot K]}$, and the specific heat capacity c_ρ is varied. In Fig. 3(b), the temperature T at the same point is shown as the function of time. As expected, the larger specific heat capacity causes the slower temperature rise since it needs more energy to raise the same amount of temperature. The numerical results agree very well with the TDFEM references, and the L_2 norm errors corresponding to $c_\rho = 300$, 500, and 700 are 1.02×10^{-4}, 1.52×10^{-4}, and 1.56×10^{-4}, respectively. Thereby, the accuracy of proposed DGTD method has been validated for both Dirichlet and convection boundary conditions.

Here, the number of mesh elements is 4530, the CPU time of each time marching step is around 0.0052 s, and the peak memory cost is around 0.01 GB.

B. 3-D Integrated System With Equivalent Thermal Parameters

In this example, a 3-D integration structure shown in Fig. 4 is investigated, where the geometrical details and material properties are given in Table I. Instead of directly considering the physical presence of TSVs and ball grid array,

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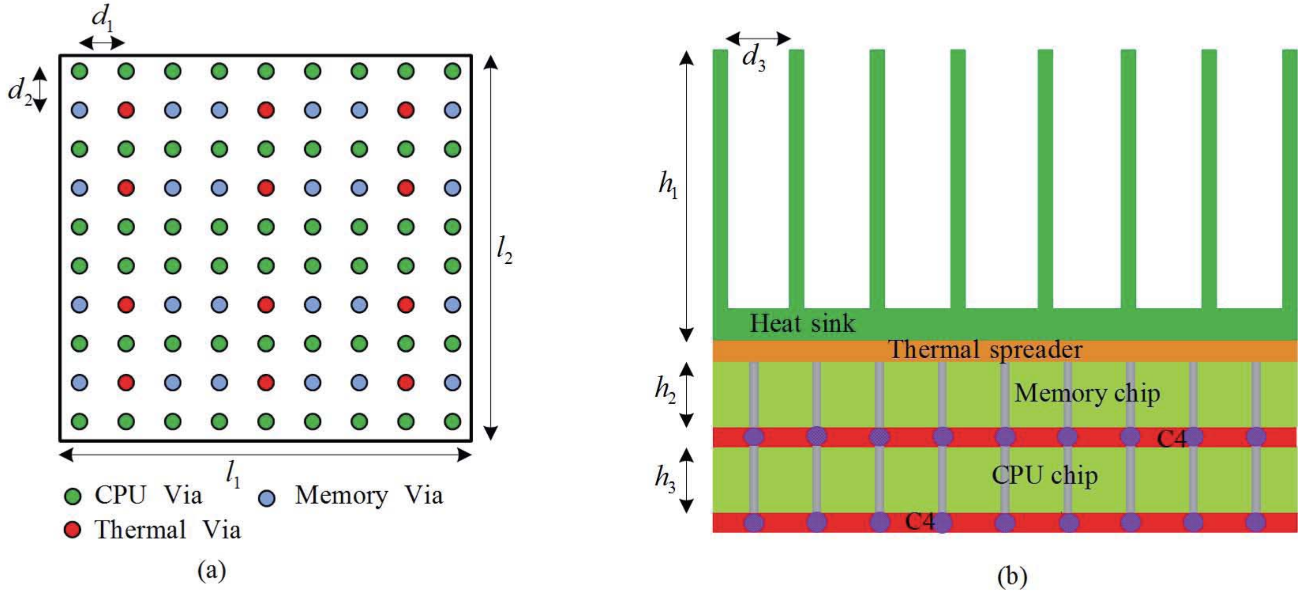

Fig. 7. Geometrical details of the investigated 3-D package. (a) Distribution of different vias. (b) Cross-sectional view of the package. The geometrical parameters are given as $l_1 = 12$ mm, $l_2 = 12$ mm, $d_1 = 1.25$ mm, $d_2 = 1.25$ mm, $d_3 = 1.95$ mm, $h_1 = 7$ mm, $h_2 = 0.5$ mm, and $h_3 = 0.5$ mm. The thickness of thermal spreader is 0.2 mm as well as C4.

TABLE II
MATERIAL PROPERTIES REQUIRED BY THE THERMAL ANALYSIS

···	κ W/[m·K]	c_m J/[kg·K]	ρ kg/m^3
Thermal Spreader	400	385	8933
Heat Sink	220	896	2707
Chip Die	135	704	2330
TSV	400	385	8933
C4	50	180	9290

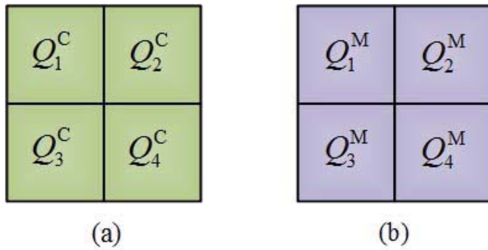

Fig. 8. Power map over (a) CPU die and (b) memory die, where $Q_1^C = 20Q_c$, $Q_2^C = 30Q_c$, $Q_3^C = 35Q_c$, $Q_4^C = 25Q_c$, $Q_1^M = 60Q_m$, $Q_2^M = 70Q_m$, $Q_3^M = 65Q_m$, and $Q_4^M = 63Q_m$ with $Q_c = \|\cos(2\pi y/3l_1)\|$ and $Q_m = \|\cos(3\pi y/2l_1)\|$.

the thermal effects of TSVs in the interposer and ball grid array in the microbump layer are equivalently replaced by revising the thermal parameters of materials in the corresponding layer [27]. In this way, the homogeneous meshes can be employed to model this structure, which consequently results in only 15 208 elements. The power consumption on dies is a Gaussian pulse defined by $Q = Q_0\exp[-(t - 1.2)^2/0.36]$ W/m^3 with $Q_0 = 3.6 \times 10^8$ on the first die and $Q_0 = 2.4 \times 10^8$ on the second die. The isotherm boundary of 298.15 K is applied to the top surface of the TIM as the heat sink, while the convection boundary with $h = 5$ W/[m$^2 \cdot$ K] is applied to the remaining surfaces of the package.

To verify the accuracy of the proposed algorithm, the transient temperature at three observation points $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_3$ with $\mathbf{r}_1 = 0.015\hat{\mathbf{x}} + 0.015\hat{\mathbf{y}} + 0.007\hat{\mathbf{z}}$, $\mathbf{r}_2 = 0.017\hat{\mathbf{x}} + 0.017\hat{\mathbf{y}} + 0.008125\hat{\mathbf{z}}$, and $\mathbf{r}_3 = 0.031\hat{\mathbf{x}} + 0.031\hat{\mathbf{y}} + 0.008125\hat{\mathbf{z}}$ located at the interposer layer, the center of first and second dies, respectively, are computed as shown in Fig. 5. For comparison, the solutions simulated by the commercial software COMSOL [28] are also presented. As can be seen, the calculated numerical results agree very well with the references. For further verification, the temperature distribution over the top surface of the interposer at $t = 2$ s is calculated and plotted in Fig. 6. As can be seen, the calculated result from DGTD algorithm associates with the reference from the COMSOL simulation [28].

In this example, the CPU time of each time-step is 0.019 s, and the memory cost is around 0.06 GB.

C. 3-D Integration Package and Interconnect

To further demonstrate the capability of the proposed algorithm for analyzing complicated multiscale systems, a 3-D integrated circuit package with vertically stacked-up chips connected by TSVs is studied, as shown in Fig. 7. This module is composed of one CPU chip and one memory die, 12 thermal vias, 54 TSVs in the CPU layer, 24 TSVs in the memory layer, a thermal spreader, and a heat sink. In Table II, the thermal equation required parameters are listed. Unlike the second example, all the geometrical elements here are modeled rigorously without using the equivalent thermal parameters. It is supposed that the convection boundary is applied at the surface of the heat sink with $h = 50$ W/[m$^2 \cdot$ K], and other surfaces are assumed to be adiabatic

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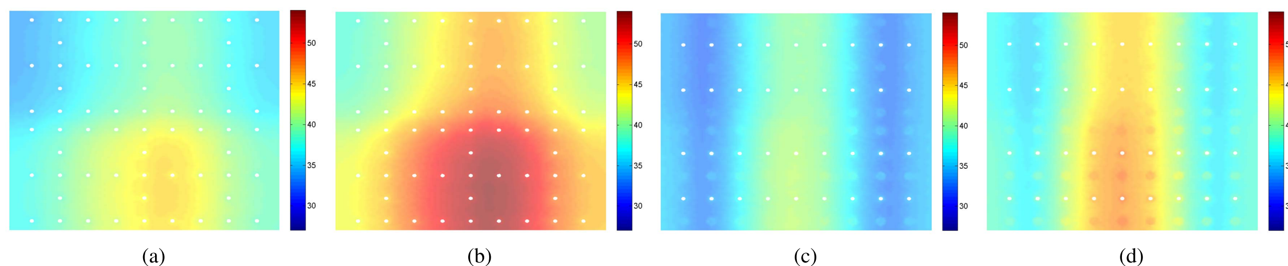
(a) (b)

(c) (d)

Fig. 9. DGTD calculated temperature distributions (°C) of the 3-D integrated circuit at (a) $t = 0.0138$ s, (b) $t = 0.02$ s, (c) $t = 0.0242$ s, and (d) $t = 0.027$ s.



(a) (b) (c) (d)

Fig. 10. (a) and (b) Temperature profiles (°C) over the bottom surface of the CPU die at $t = 0.02$ s and $t = 0.027$ s, respectively. (c) and (d) Temperature profiles over the bottom surface of the memory die at $t = 0.02$ s and $t = 0.027$ s, respectively.

(The convective heat transfer coefficient $h = 0$ W/[m$^2 \cdot$ K]). The heat power consumptions of the CPU and memory dies are described in Fig. 8, while a 50-W impressed heat source is placed over the thermal spreader. Totally, 469 220 strongly inhomogeneous tetrahedrons are generated, which results in 7 507 520 unknowns. Even though there are more than seven million unknowns, in the DGTD analysis, the dimension of the matrix equation for factorization is 4 by 4 since the DGTD method in this paper solves the whole computational domain in an element-by-element scheme. Thus, it is free of issues encountered in the FEM such as factorization of a very large matrix (the dimension of the global matrix is a few millions) that could be seriously ill-conditioned due to the very inhomogeneous mesh cells.

In Fig. 9, the 3-D temperature profiles at $t = 0.0138$ s, $t = 0.02$ s, $t = 0.0242$ s, and $t = 0.027$ s obtained from the proposed DGTD algorithm are provided. The 2-D temperatures at the bottom surfaces of the CPU die and memory die at $t = 0.02$ s and $t = 0.027$ s are plotted in Fig. 10. It is interestingly noted that the temperature of the memory die raises slowly compared to the CPU die although the power consumption in the memory die is higher, which is attributed to the memory die attached with the thermal spreader so that the generated heat can be transferred to the heat sink.

Finally, consider that the above heat sources are modulated by a pulse $G_0(t)$ shown in Fig. 11. The transient temperature variations at different positions over the chip

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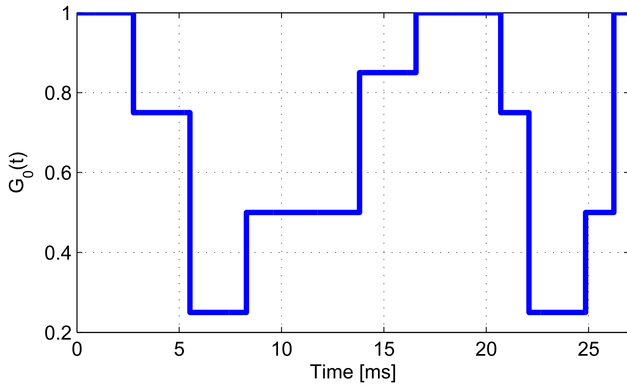

Fig. 11. Pulse $G_0(t)$ used to modulate the heat source.

TABLE III
CORRESPONDING SPATIAL COORDINATES (mm) FOR THE CURVES IN FIG. 12

···	r_1	r_2	r_3	r_4	r_5	r_6
x	0.1934	-4.8852	-5.0297	-5.0297	-3.5006	-1.4872
y	0.0013	0.0007	-3.0952	-3.0952	-2.8667	4.8062
z	0.3547	0.1693	0.3022	0.3022	0.9162	0.9166

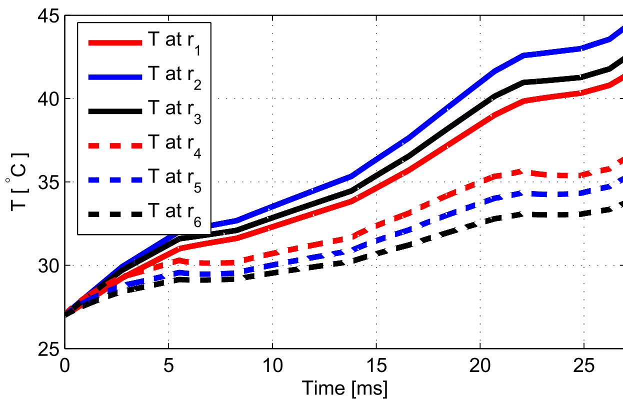

Fig. 12. Transient temperature profiles (°C) at different positions listed in Table II.

die and memory die listed in Table III are plotted in Fig. 12.

For this example, the CPU time of each time marching step is around 0.7 s, and the peak memory cost is around 1.52 GB.

IV. CONCLUSION

A DGTD algorithm is developed in this paper for analyzing the heat transfers in 3-D integrated circuits and packages. To solve the parabolic heat equation by the DGTD method, an auxiliary vector named heat flux is introduced that degenerates the parabolic one to a hyperbolic equation. Due to the local operation of DGTD, the whole computational domain can be solved in an element-by-element scheme. Thus, it is free of issues such as the factorization of a huge matrix equation that is usually ill-conditioned due to multiscale meshes. The proposed algorithm is verified both analytically and numerically, as well as its capability to handle multiscale structures.

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