NanoLeak: A Fast Analytical Green's Function-based Leakage-aware Thermal Simulator

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Abstract— In this paper, we propose *NanoLeak*, a comprehensive temperature simulator that incorporates both classical heat transfer mechanisms and nanoscale effects. It performs both steady state and transient analyses while automatically taking leakage into account. We derive closed-form expressions for the Green's function (impulse response of a power source) for all scenarios with leakage; there is no need for the traditional, time-consuming iterative solutions. We show a speedup of 1250X for the classical heat transfer case (Fourier's heat equation) with an error limited to 2.4% in computing the steady-state thermal profile. At nanoscale levels, the Boltzmann transport equation (BTE) is solved to analyze the temperature profile. In this paper, we analytically compute the leakage-aware solution for the gray-BTE model and compare the results against competing, state-of-the-art work (211-2580X speedup).

Keywords*— *Temperature modeling, Green's function, Nanoscale effects

I. Introduction

It is widely accepted that temperature is a first-order design criterion in the design of processors. Temperature simulation is done at various stages of the design flow, albeit with different amounts of information. For example, designers get a rough idea of the final temperature at the architecture design or floorplanning stage itself such that high-level decisions can be made and the broad contours of the cooling solution can be worked out. Temperature estimation is later done after the design is synthesized to get an even more accurate idea of the final thermal profile of the chip. This helps tune different power management mechanisms. Given that there is a leakage-temperature feedback loop, temperature hotspots further exacerbate the problem and have a detrimental effect on the ultimate reliability of the chip.

The area of temperature estimation methods for processors is very well-established. Typically, using classical techniques such as finite element (FEM) or finite difference (FDM) approaches is very slow. It is often necessary to run thousands of temperature simulations [1,2]; consequently, fast simulation times with low error become necessary. As a result, Green's function-based approaches [3] have achieved prominence in the last few years. A Green's function is defined as the impulse response of a unit power source, and computing the temperature profile is as simple as convolving the power profile with the Green's functions (with some corrections at the edges and corners). Such approaches are several orders of magnitude faster than competing approaches that are derived from finite difference based approaches [4].

Unfortunately, for modern sub-10 nm technologies, solving traditional heat equations (Fourier equations) is not enough. We need to take nanoscale effects such as phonon transport as well [5,6], particularly as the technology node starts to reduce beyond the mean free path of phonons (beyond 45nm). We need to solve the gray-BTE equation [7] to compute the temperature profile of such devices. Most existing thermal simulators [1,2,8] do not take this into account, leading to an error of 25-60% in temperature estimation [5,6,9].

A recent paper by Varshney et al. [9] titled *Nanotherm* has addressed this issue and proposed a Green's function-based approach for solving both the classical Fourier's heat equation and the gray-BTE equation. In their paper, the authors report a substantial speedup over existing FEM-based approaches. However, this paper is **incomplete** in the sense that the authors do not model leakage power or the leakage-temperature feedback loop. Particularly, when we consider phonon transport mechanisms computing leakage power is of paramount importance. The increased temperature does manifest in greater localized leakage power, and this needs to be modeled and aggregated. To use the *Nanotherm* model for modeling leakage power, it is necessary to run the model once, update the temperature, compute the leakage power, run it once again, and so on, until convergence. This is a time-taking, iterative process and in our experiments at least 4-5 iterations were required. Again, the temperature does not converge at all points; there are always a few points that demand more iterations.

We adopt a more direct approach in this paper, where we bring in leakage directly into the analytical expression of the Green's function. We start with the equations

TABLE I
Comparison of thermal simulators

Simulator	Fourier	Leakage aware Fourier	BTE	Leakage aware BTE
COMSOL	✓	✗	✗	✗
ThermalScope	✓	✗	✓	✗
HotSpot [1]	✓	✗	✗	✗
3DICE [2]	✓	✗	✗	✗
NanoTherm [9]	✓	✗	✓	✗
NanoLeak	✓	✓	✓	✓

proposed in *NanoTherm* and then extend them to automatically incorporate the effects of leakage. This is not a simple extension, and it turned out to be quite non-trivial. The advantage is that for both classical thermal analyses (Fourier's equations) and analyses based on the gray-BTE equation, there is no need to go for a tedious, iterative process. We can directly use the modified equations and then convergence at all the points is guaranteed. There is a direct speedup in terms of the computational time vis-a-vis *NanoTherm* and we also avoid the numerical precision issues that typically bedevil such approaches that rely on convergence. The theoretical techniques presented in this paper can possibly be used in other problems of a similar nature. Table I summarizes the design space.

We discuss the relevant background in Section II. Next we present our methodology in Section III. We finally proceed to discuss the evaluation in Section IV and conclude in Section V.

II. Background

A. Fourier's Heat Equation

Heat transfer in solids is governed by the Fourier's heat equation (Equation 1). This equation is valid for cases where the geometry of the device is much larger than the mean free path of phonons. It does not model the quantum effects prevalent in nanoscale devices.

$$\rho c \frac{\partial T}{\partial t} - k\nabla^2 T = q_{vol} \tag{1}$$

Here, ρ is the density, c is the specific heat, k is the thermal conductivity, q_{vol} is the volumetric heat, T is the temperature profile and t is the time. Equation 1 is solved using FEM/FDM based methods [1, 8] or using Green's function-based methods [3].

B. Boltzmann Transport Equation

Phonons, which are quantized lattice vibrations, play a crucial role in determining the temperature distribution at the nanometer scale. They exhibit wave-particle duality. In nanoscale devices, the mean free path of phonons becomes comparable with the dimensions of the devices under consideration [6]. In such cases, the wave nature of phonons cannot be neglected. Hence, the Fourier's heat equation fails. To model the phonon effects, we solve the Boltzmann transport equation(BTE) [10]. Typically, we solve this equation by taking the Gray approximation, which assumes that all the phonons are grouped at the same frequency node with the same group velocity and relaxation time. It is a widely accepted model (refer to Equation 2).

$$\frac{\partial e_\omega}{\partial t} + \overrightarrow{v_g} \cdot \nabla e_\omega - \frac{Q}{4\pi} = \left(\frac{\partial e_\omega}{\partial t}\right)_{collision} \tag{2}$$

where e_ω is the energy density per unit solid angle, $\overrightarrow{v_g}$ is the group velocity of phonons, t is the time, and Q is the volumetric heat generation. The RHS term models the phonon scattering.

C. Leakage power

The leakage power is exponentially dependent on temperature and can be modeled using the simplified BSIM4 equation [11] given by Equation 3.

$$P_{leak} = v_T^2 * e^{\frac{V_{GS} - v_{th} - v_{off}}{\eta v_T}} (1 - e^{\frac{-V_{DS}}{v_T}}) \tag{3}$$

Here, v_T is the thermal voltage, v_{th} is the threshold voltage, v_{off} is the offset voltage in the sub-threshold region and η is a constant. Experiments done in [12, 13] have shown that over the operating temperature range of ICs, the leakage power can be assumed to be linearly dependent on temperature. Also, in [14], the authors have shown that the linear leakage model provides an accuracy of over 96%, which is sufficient for the early design and architectural exploration stages. Hence, we simplified linear model to calculate the leakage power. This approach has been used in other works as well [15, 16].

D. Green's Function

The Green's function is defined as the impulse response of a unit power source (Dirac delta function) applied to the center of the chip. During the pre-compute stage, the Green's function is computed and stored. It is then used to quickly compute the temperature profile of the chip at runtime.

$$T = G \star P \tag{4}$$

where, G is the Green's function, P is the power profile of the chip, and $\star$ is the convolution operator. Green's function based methods are significantly faster compared to conventional FEM/FDM based approaches [3, 4].

E. Hankel Transform

For a radially symmetric function, a 2D Fourier transform is analogous to a zero-order 1D Hankel transform.

$$\mathcal{H}(\sigma) = \mathcal{H}(f(r)) = \int_0^\infty r f(r) \mathcal{J}_0(\sigma r) dr \tag{5}$$

where, $\mathcal{H}$ is the Hankel operator, $\mathcal{J}_0$ is the zero-order Bessel function of the first kind, r is in the polar coordinates and σ is the Hankel variable.

TABLE II
GLOSSARY

Symbol	Meaning
ϕ_s	Analytical Green's function
q_0	Volumetric heat source
r_0	Radius of the heat source
k_1	Thermal conductivity of the chip
J_1	Bessel function of the first kind
σ	Hankel domain variable
z	Position in the z direction
b	Thickness of the heat spreader
δ	Thickness of the silicon die
$\mathcal{T}$	Transient leakage-aware temperature profile

III. Methodology

A. Fourier Analysis

The Fourier's heat equation given by Equation 1 is solved to obtain the Green's function of a chip. This can be done either using FEM/FDM or by using analytical methods (as done in [9]).

1. Steady State

The calculated Green's function without considering the effects of leakage in the Hankel domain is given by [9],

$$\phi_s(\sigma, z) = \frac{q_0 r_0}{k_1} \frac{J_1(r_0\sigma)}{\sigma^2} \frac{1}{1 - f(\sigma)} (e^{-\sigma z} + f(\sigma) e^{\sigma z}) \quad (6)$$

where,

$$f(\sigma) = e^{-2\sigma\delta} \frac{k_1 tanh(b\sigma - k_2)}{k_1 tanh(b\sigma + k_2)} \quad (7)$$

Table II describes the relevant parameters.

Let us consider the two components of power: the dynamic power P_{dyn} and the leakage power P_{leak}. From Equation 4, the complete temperature profile of the chip is thus given by,

$$T = f_s * (P_{dyn} + \Delta P_{leak}) \quad (8)$$

where, f_s is the Green's function without leakage.
In our analysis, we consider a linear model for leakage, which is given by Equation 9

$$\Delta P_{leak} = \beta T \quad (9)$$

where, β is a constant depending on the properties of the chip. It is given by $\beta = \frac{dP_{leak}}{dT}$. Hence, Equation 8 becomes,

$$T = f_s * P_{dyn} + \beta (f_s * T) \quad (10)$$

Next, we take the 2D Fourier Transform on both sides. To simplify our analysis, we use the Hankel transform. The Hankel transform of a 2D function is equal to the product of the transforms scaled by the factor of 2π. Taking the Hankel transform, we get

$$\mathcal{H}(T) = \mathcal{H}(f_s) + 2\pi\beta \mathcal{H}(f_s)\mathcal{H}(T) \quad (11)$$

$\mathcal{H}(f_s)$ is the analytically computed Green's function ϕ_s. Taking $\mathcal{H}(T)$ to the LHS, we get the leakage-aware steady state Green's function,

$$\boxed{\mathcal{H}(T) = \frac{\phi_s}{1 - 2\pi\beta\phi_s}} \quad (12)$$

2. Transient Analysis

To incorporate the effect of variations in the temperature profile with time, we add a capacitive term to the steady state equation [16]; the resultant equation becomes,

$$\mathcal{T} = f_s + \beta f_s * \mathcal{T} - C f_s \frac{d\mathcal{T}}{dt} \quad (13)$$

By following the same steps as we followed to derive the steady state response, together with the condition $2\pi\beta\mathcal{H}(f_s) \ll 1$, we get

$$\mathcal{H}(\mathcal{T}) = \mathcal{H}(f_s)(1+2\pi\beta\mathcal{H}(f_s)) - 2\pi C \mathcal{H}(f_s)\mathcal{H}\left(\frac{d\mathcal{T}}{dt}\right)(1+2\pi\beta\mathcal{H}(f_s)) \quad (14)$$

The first term in Equation 14 can be approximated as the steady state leakage aware Green's function ϕ_{sleak}. Let $f_\alpha = 2\pi C(1 + 2\pi\beta\mathcal{H}(f_s))$. Equation 14 reduces to

$$\mathcal{H}(\mathcal{T}) = \phi_{sleak} - f_\alpha \mathcal{H}(f_s)\mathcal{H}\left(\frac{d\mathcal{T}}{dt}\right) \quad (15)$$

This is a first order linear differential equation. Applying the boundary condition $\mathcal{H}(\mathcal{T})|_{t=0} = 0$ and solving, we get

$$\mathcal{H}(\mathcal{T}) = \phi_{sleak} - \phi_{sleak} e^{\frac{-t}{f_\alpha \mathcal{H}(f_s)}} \quad (16)$$

Let us compute the inverse Hankel transform of Equation 16. The first term is the steady state temperature profile $\mathcal{T}_{ss}$. Let the second term be $finv$.

$$\mathcal{T} = \mathcal{T}_{ss} - finv \quad (17)$$

Let us separate $finv$ into two parts: $finv_0^\epsilon$ and $finv_\epsilon^\infty$. $finv_\epsilon^\infty$ is the value of $finv$ between ϵ and ∞. It is thus given by,

$$finv_\epsilon^\infty = \int_\epsilon^\infty \phi_{sleak} e^{\frac{-t}{2\pi C \phi_{sleak}}} J_0(\sigma r)\sigma d\sigma \quad (18)$$

$finv_0^\epsilon$ is the value of $finv$ between 0 and ϵ. When $\epsilon \to 0$, $\sigma r = 0$, and $J_0(\sigma r) = 1$. When $\sigma \to \epsilon$, $f_\alpha = f_0 = 2\pi C(1 + 2\pi\beta\mathcal{H}(f_s)|_{\sigma=0}$.
Also, since $\frac{\delta(\sigma)}{\sigma} \gg \beta\mathcal{T}$, we can ignore the leakage terms present in ϕ_{sleak}. Hence, we can approximate $\mathcal{H}(\mathcal{T}_{ss}) = \mathcal{H}(f_s) = \mathcal{H}(f_s)|_{\sigma=0}\frac{\delta(\sigma)}{\sigma}$. Thus, $finv_0^\epsilon$ becomes

$$finv_0^\epsilon = \int_0^\epsilon \mathcal{H}(f_s)|_{\sigma=0} \frac{\delta(\sigma)}{\sigma} e^{\frac{-t}{f_0 \mathcal{H}(f_s)|_{\sigma=0}\frac{\delta(\sigma)}{\sigma}}} \sigma d\sigma \quad (19)$$

$$finv_0^\epsilon = \frac{(\mathcal{H}(f_s)|_{\sigma=0})^2 f_0}{\epsilon^2 t}(1 - e^{\frac{-t\epsilon^2}{f_0 \mathcal{H}(f_s)|_{\sigma=0}}}) \quad (20)$$

The transient leakage-aware temperature profile becomes

$$\boxed{\mathcal{T} = \mathcal{T}_{ss} - finv_0^\epsilon - finv_\epsilon^\infty} \quad (21)$$

TABLE III
GLOSSARY

Symbol	Meaning
Q	Volumetric heat generation
τ	Phonon relaxation time
Λ	Mean free path
ξ_x,ξ_y,ξ_z	Spatial frequency in the x,y, and z directions
C	Specific heat
f_{sp}	gray-BTE solution
$\mathcal{F}$	Fourier transform
η	Temporal frequency

B. BTE Analysis

The gray-BTE equation is analytically solved in [9] to obtain the Green's function. We modify it to incorporate leakage.

1. Steady State

The Green's function for the steady state gray BTE is as follows.

$$\mathcal{F}(f_{sp}) = \frac{\widetilde{Q}\tau}{C}\frac{\frac{1}{\Lambda\xi}\tan^{-1}(\Lambda\xi)}{1-\frac{1}{\Lambda\xi}\tan^{-1}(\Lambda\xi)} \tag{22}$$

Table III describes the relevant parameters. The temperature field $\mathcal{U}$ of the device considering leakage is given by

$$\mathcal{U} = f_{sp} \star (P_{dyn} + \Delta P_{leak}) \tag{23}$$

where, $\xi = \sqrt{\xi_x^2 + \xi_y^2 + \xi_x^2}$. Considering a linear leakage model, $\Delta P_{leak} = \beta\mathcal{U}$ and P_{dyn} as the Dirac delta function (a point source with 1 W power), we get

$$\mathcal{U} = f_{sp} + \beta f_{sp} \star \mathcal{U} \tag{24}$$

Computing the 2D fourier transform of the LHS and RHS and rearranging the terms, we get the steady state Green's function considering leakage in the Fourier transform domain

$$\mathcal{F}(\mathcal{U}) = \frac{\mathcal{F}(f_{sp})}{1-\beta\mathcal{F}(f_{sp})} \tag{25}$$

where, $\widetilde{X}$ stands for the Fourier transform of variable X. Putting the value of $\Delta\widetilde{T}$ in Equation 25 and solving it we get the leakage-aware steady state Green's function for the gray-BTE model.

$$\boxed{\mathcal{F}(\mathcal{U}) = \frac{\widetilde{Q}\tau}{C}\frac{\frac{1}{\Lambda\xi}\tan^{-1}(\Lambda\xi)}{1-\frac{1}{\Lambda\xi}\tan^{-1}(\Lambda\xi)(1+\beta\frac{\widetilde{Q}\tau}{C})}} \tag{26}$$

2. Transient Analysis

The transient Green's function for gray BTE without considering leakage (as calculated in [9]) is given by Equation 27.

$$\mathcal{F}(f_{sp}) = \frac{\widetilde{Q}\tau}{C}\frac{\frac{1}{\Lambda\xi}\tan^{-1}\left(\frac{\Lambda\xi}{1+i\eta\tau}\right)}{1-\frac{1}{\Lambda\xi}\tan^{-1}\left(\frac{\Lambda\xi}{1+i\eta\tau}\right)} \tag{27}$$

Following a similar procedure, we get the transient leakage-aware Green's function to be as follows.

$$\boxed{\mathcal{F}(\mathcal{U}) = \frac{\widetilde{Q}\tau}{C}\frac{\frac{1}{\Lambda\xi}\tan^{-1}\left(\frac{\Lambda\xi}{1+i\eta\tau}\right)}{1-\frac{1}{\Lambda\xi}\tan^{-1}\left(\frac{\Lambda\xi}{1+i\eta\tau}\right)(1+\beta\frac{\widetilde{Q}\tau}{C})}} \tag{28}$$

IV. Evaluation

A. Setup

We ran the Fourier simulations on an Intel $i3$ laptop with $4GB$ RAM running Windows 10. The BTE simulations were run on an Intel $i7$ desktop with $12GB$ RAM running Ubuntu 16.01 LTS. We used the commercial CFD simulator COMSOL(version 5.5) to validate the Fourier results. For BTE validation, we used the FEM-based ThermalScope (ISAC2) tool. The Fourier analysis scripts were written in R 3.6.1 and the BTE scripts were written in MATLAB2020b. **All our results take leakage into account.**

B. Fourier Analysis

For the Fourier analysis, we consider a 11.2 mm × 11.2 mm × 0.15 mm chip with a 11.2 mm × 11.2 mm × 3.52 mm heat spreader placed on top of it. The thermal conductivity of the chip and the heat spreader are taken to be 150 W/mK and 256 W/mK, respectively. To compute the Green's function, we need a circular power source at the center of the chip. But we can simulate only rectangular/square elements in a real chip. Hence, we mapped square sources to circular sources as suggested in [9]. Next, we discretize the chip into 0.2 mm × 0.2 mm blocks, which was found to be sufficient in other works as well [9]. The percentage errors reported for Fourier analysis are with respect to the maximum temperature rise.

1. Steady State Analysis

We compare the Fourier steady-state Green's function as per our results versus COMSOL in Figure 1. The error in computing the maximum temperature rise was observed to be 2.4 %. Our system takes a total time of 1.22 s to compute the Green's function for a 11.2 mm × 11.2 mm chip. To compute the Green's function, we build the same model configuration in COMSOL with a 0.2 mm × 0.2 mm heat source at the center. To compute the leakage aware temperature profile in COMSOL, we run the thermal simulation multiple times till the leakage power and temperature values converge; this takes approximately 25 min. We thus achieve a speedup of 1250X over a commercial CFD simulator.

2. Transient Analysis

We run the transient Fourier simulation for the same setup as before. Figure 2 shows the step response for 100 radial points and 100 time steps. This takes approximately 2.24 min. The total runtime of our algorithm for one time step is 1.62 s, as compared to 45 min (speedup of 1670X) taken by COMSOL, with the error limited to

2 %.

Full-chip thermal profile: We also compute the full-chip (Intel Gainestown) temperature profile (same setup as [9]) using our algorithm for both the steady state and transient case, respectively. We show the simulation results for only one test case due to space constraints. In Figure 4, we show the transient full-chip thermal profile for a random power map at time steps of 1 ms, 5 ms, and 10 ms, respectively. This takes approximately 1.62 s.

C. BTE Analysis

We compare the leakage-aware BTE solution against the state-of-the-art tool ThermalScope for a 60 nm × 45 nm × 20 nm channel FET [5, 6]. The values of various constants in the BTE equation are taken from ThermalScope.

1. Steady State Analysis

We run the steady-state BTE simulation for the device configuration described above. We observe a simulation time of 4.3 s for 400 × 400 × 200 grid points. Next, we run ThermalScope for 60 × 60 × 48 grid points. For leakage-aware analysis in ThermalScope, we need to perform the simulation multiple times till the leakage power and temperature values converge. This takes approximately 185 min. Hence, we achieve a speedup of 2580X over ThermalScope with an RMS error of 0.05 °C. Note that *NanoLeak* considers far more points (400 × 400 × 200) as compared to ThermalScope. Figure 5 shows the comparison of ThermalScope with *NanoLeak* for steady state simulation.

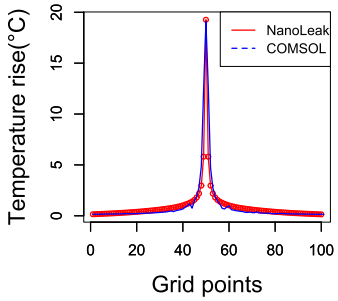


Fig. 1. Comparison of Fourier steady state simulation results with COMSOL

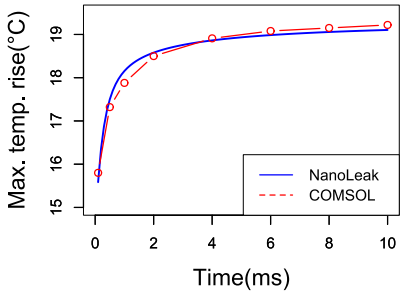


Fig. 2. Comparison of Fourier transient simulation results with COMSOL

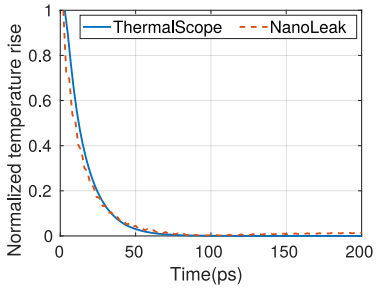


Fig. 3. Comparison of ThermalScope with *NanoLeak* for BTE transient simulation

2. Transient Analysis

We run a transient simulation for the same configuration. We observe a simulation time of 68 s for 200 time steps. Next, we run ThermalScope for 60 × 60 × 48 grid points; the total simulation time was 244 min (speedup of 211X). The RMS error, in this case, was 0.053 °C (see Figure 3).

D. Simulation Speed

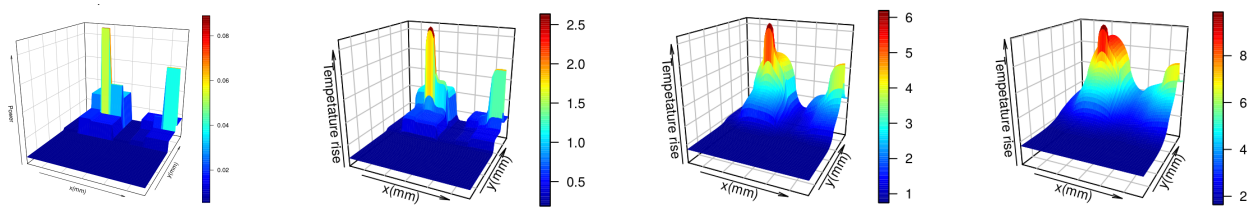
Table IV summarizes the time taken to compute the Green's function for various commercial thermal simulators and our approach *NanoLeak*. Our algorithm is 1250 times faster in computing the steady state Fourier solution as compared to COMSOL. For transient simulation, we show a speedup of 1670X. We are 2580 times faster than ThermalScope in computing the steady state BTE solution, and 211 times faster in calculating the transient solution. We also compare our algorithm against *Nanotherm*. It typically takes 4-5 iterations for computing the leakage-converged thermal profile, but it faces convergence issues, especially for the BTE simulations. *NanoTherm* is faster for the Fourier steady-state case because they use an approximation in their code (omit computing a term), which we cannot use.

V. Conclusion

In this paper, we proposed an ultra-fast thermal simulator *NanoLeak* that takes both the leakage effects and nanometer-scale level effects into account. As compared to the commercial CFD simulator COMSOL, we observe a speedup of 1250X in computing the Fourier steady state Green's function with the error being 2.4 % and a speedup of 1670X with an error less than 2 % for transient simulation. We also compare the leakage-aware BTE solution with the state-of-the-art tool ThermalScope. We achieve

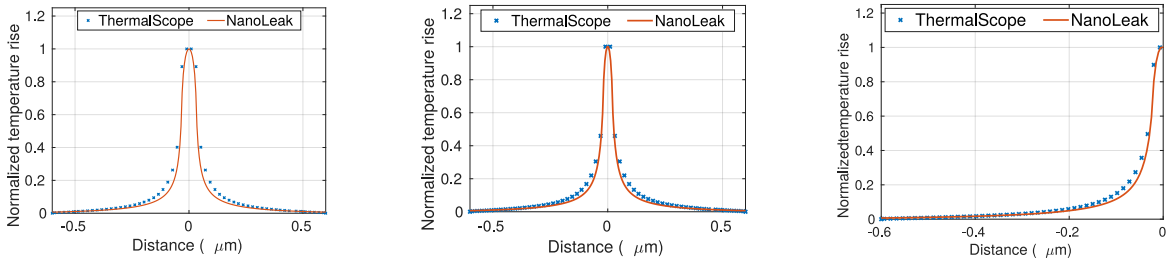
TABLE IV
Speed of thermal simulators

Simulator	Fourier heat eq.		BTE	
	Steady	Transient	Steady	Transient
COMSOL	1500 s	2880 s	-	-
ThermalScope	-	-	185 min	240 min
NanoTherm	0.415 s	16.8 s	16.5 s	158 s
NanoLeak	1.22 s	1.62 s	4.3 s	68 s



(a) Power distribution (b) ΔT at 1ms (c) ΔT at 5ms (d) ΔT at 10ms

Fig. 4. Transient full-chip thermal profile (Intel Gainestown die, refer to [9])



(a) Along x axis (b) Along y axis (c) Along z axis

Fig. 5. Comparison of ThermalScope with *NanoLeak* for BTE steady state simulation

a speedup of 2580 times with an RMS error of 0.5 °C. For transient simulation, we achieve a speedup of 211X with an RMS error of 0.0527 °C.

Acknowledgement

This work was supported in part by the Semiconductor Research Corporation (SRC).

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