Enhanced Operator Learning for Scalable and Ultra-fast Thermal Simulation in 3D-IC Design

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ABSTRACT

Thermal simulation plays a critical role in the design of 3D integrated circuits (3D-ICs), where accurate and efficient temperature predictions are essential to ensure component reliability and performance. Recently, deep learning methods have shown great potential in accelerating these simulations. **DeepOHeat** [1] is one such approach, designed to learn solution operators that map single or multiple configurations of heat equations—such as surface power, volume power, or heat transfer coefficients—directly to the 3D temperature distribution. By utilizing a physics-informed DeepONet framework[2], DeepOHeat effectively captures complex relationships between design parameters and temperature fields, even when no training data is available and only PDE constraints are imposed.

As a specific example, DeepOHeat can model the steady-state heat conduction problem where the surface power input q_n is mapped to the temperature field $T(\boldsymbol{y})$. This is expressed through the following neural operator approximation:

$$T_{\boldsymbol{\theta}}(q_n)(\boldsymbol{y}) = b_\psi(\mathcal{E}(q_n)) \cdot t_\phi(\boldsymbol{y}), \tag{1}$$

where $\mathcal{E}$ is a function encoder mapping q_n to point-wise evaluations, and b_ψ and t_ϕ are fully-connected neural networks (the branch and trunk nets, respectively). As demonstrated in [1], DeepOHeat has achieved excellent accuracy in predicting the temperature profiles of realistic chip designs. Once trained, DeepOHeat can provide real-time temperature predictions for unforeseen power maps.

Despite its strong predictive accuracy, the scalability of DeepOHeat is limited due to the high computational cost associated with dense sampling of collocation points for physics-informed optimization across multiple design configurations.

To address these limitations, we introduce **DeepOHeat+**, which incorporates the Separable Operator Network (SepONet) [3] to enhance scalability. DeepOHeat+ leverages low-rank functional approximation to factorize the trunk network into independent univariate trunk nets, significantly reducing computational complexity. The temperature field is approximated as:

$$T_{\boldsymbol{\theta}}(q_n)(\boldsymbol{y}) = b_\psi(\mathcal{E}(q_n)) \cdot \left(t^1_{\phi_1}(y_1) \odot t^2_{\phi_2}(y_2) \odot t^3_{\phi_3}(y_3)\right), \tag{2}$$

where $\odot$ denotes the Hadamard (element-wise) product. This separability allows for faster, more memory-efficient training via forward-mode automatic differentiation, compared to DeepOHeat's single multivariate trunk net.

Our results, based on the surface power example, demonstrate that **DeepOHeat+** significantly improves training efficiency compared to DeepOHeat. As shown in Table 1, DeepOHeat+ achieves a 64x reduction in training time, requiring only 3.05ms per iteration, and reduces GPU memory usage by 31x, using only 0.56GB. In contrast, DeepOHeat requires 197.73ms per iteration and 17.73GB of GPU memory. Despite these improvements in efficiency, DeepOHeat+ maintains comparable accuracy, achieving a relative ℓ_2 error of 1.65%, similar to DeepOHeat's 1.86% when evaluated on 10 new surface power configurations. These results highlight the scalability of DeepOHeat+ for thermal simulations in 3D-IC design, offering substantial computational savings without sacrificing accuracy.

Table 1: Comparison of DeepOHeat and DeepOHeat+ in terms of efficiency and accuracy.

Models	Training Time	GPU Memory	Rel. ℓ_2(%)
DeepOHeat	197.73ms/iter	17.73GB	1.86
DeepOHeat+	3.05ms/iter (64× ↓)	0.56GB (31 × ↓)	1.65

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