AI-Enabled Development of Cooling Device for High-Power Electronics

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1. Introduction

Although Phase Change Materials (PCMs) have been in the market for decades, the recent advancement in high power electronics is accelerating the development of next generation PCM solutions to maintain electronic devices temperature at a desired target. Traditional PCMs suffer from low thermal conductivity limiting the rate at which they can absorb heat (i.e., cooling power density), and such insufficient heat transfer capability slows PCM's response to sudden spikes in heat flux, causing transient temperature rises that compromise device performance or reliability [1]. To improve heat transfer while maintaining their cooling energy density, PCMs are enhanced with thermally conductive additives (e.g., graphitic carbon [2] and metal foams [3]) and being coupled to heater spreader to get the heat from the electronic component into the PCM. However, the design of such PCM composites faces several challenges: First, the rational design of the composite requires compatibility of conductive additives and PCM. Second, the PCM-to-additive ratio must be carefully optimized, as excessive fillers can reduce energy storage capacity and material reliability, while insufficient fillers result in limited thermal conductivity improvement. Lastly, the thermomechanical stability of the composite should not be compromised.

2. Discovery Process of PCM composites

Heat spreader structures are typically designed using heuristic rules (straight, pin, or plate geometry) [4], which is a time-consuming and suboptimal design process in order to balance conduction, convection, and PCM coupling under realistic operating conditions. As a matter of fact, the design of a thermal interface between the heat spreader and the PCM composite, constitutes often the bottleneck of the entire cooling device development. This is mainly due to the trial-and-error process (see Figure 1) of creating preliminary designs using iterative computational procedures (CFD) that will be tested in the sequel via a series of simulations (FEA) and physical experiments [5], in order to assess their thermomechanical stability and manufacturability.

The AI4Cooling project between CNRS@Create and NTU of Singapore aims to develop a self-driving laboratory [6] for accelerating the design of high-performance heat sinks for transient thermal management in high-power electronics. Generative AI (GenAI) [7] will be used to learn the join distribution of topologies coupled with PCMs (Thermal, Physical, Chemical, Mechanical) and heat spreader (Geometry, Thermal, Boundary) properties [8,9]. This will allows us to explore in silico a broader design space for hypothesizing entirely novel heat spreader geometries, material distributions, and PCM-additive configurations. Graph Learning [5] will be used to implement both a forward (from PCA composites->properties) and inverse design (from properties->synthetic composites) phases (see Fig 1). In a nutshell, AI4Cooling aims to speed up by 5-10X the time needed to engineer PCM composites and reduce by at least 30% the cost of manufacturing prototypes!

3. The AI4Cooling Proposal

GenAI will serve as a hypothesis generator, proposing candidate PCM composite formulations and guiding material exploration through graph-based generative models with explainability tools. These AI-generated hypotheses are then validated and enriched through systematic PCM composite synthesis and characterization, producing high-quality datasets of thermal and mechanical properties. The curated data are subsequently used in topology optimization (TO) simulations, which discover three-dimensional, multi-material heat sink geometries that co-optimize conduction, convection, and phase-change buffering under additive manufacturing constraints. More importantly, TO results capturing optimized geometries, PCM composite distributions, and transient heat responses are fed back to GenAI as training data, enabling the AI models to learn structure–property–performance relationships and rapidly predict the performance of unexplored designs. This close loop ensures that AI does not operate in isolation but is coupled with experimental data and physics-based optimization, delivering a robust, manufacturable pathway to next-generation thermal management solutions. In essence, AI4Cooling is expected to disrupt multiple stages of traditional PCM discovery processes:

•*Design generation*: The Unified Graph representation space will allow us to train GenAI models that explicitly account for transient PCM dynamics (melting and solidification) and efficient heat conducting pathways, as well as constraints of additive manufacturing (AM). Hence, the generated designs are expected to be both thermally efficient and manufacturable.

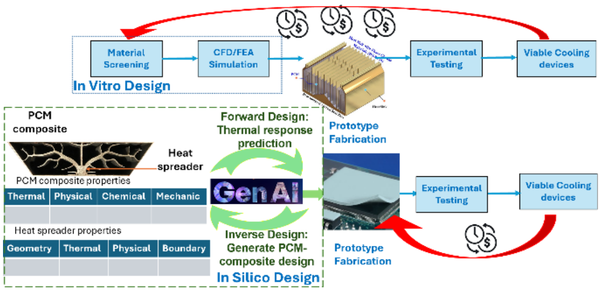

Fig. 1: Physics-based vs Generative Design of PCM Composites

•*Design validation*: Factual & Counterfactual explanation methods for graphs[15] will enable us to identify in silico critical design levels by varying the structure and properties of the generated PCM composites. This is expected to reduce the cost of screening PCM composites to achieve an optimized thermal conductivity, latent heat capacity, or thermomechanical stability.
•*Design revision*: Given the exponential and non-linear nature of the design space coupling geometry (thickness, branching, topology) and material properties (conductivity, melting range, enthalpy) as well as the sparsity of data from past experiments, unexpected synthetic composites may be systematically promoted by GenAIforces us to revise the initial design space.

4. Related Work

Existing studies on PCM composites have largely focused on improving thermal conductivity through the addition of high-conductivity fillers such as graphite, carbon nanotubes, or metal foams. While these approaches enhance heat transfer, they often suffer from reduced latent heat capacity, poor dispersion stability, and thermomechanical degradation under repeated phase-change cycles. Most prior works report trade-offs between thermal conductivity enhancement and cooling energy density, without systematically balancing both. AI4Cooling will advance the sota by systematically engineering PCM composites with simultaneously optimized latent heat capacity, thermal conductivity, and mechanical robustness. Rigorous characterization methods are required to establish a holistic property-performance map and ensure that the composites not only achieve high cooling energy density and power density but also maintain structural and thermal stability over extended cycling, positioning them as practical candidates for AM-enabled heat sink applications.
Graph Diffusion Models (GDM) [11] performance excellence was demonstrated in the literature on unconditional generation, without considering any graph constraints required to account additive manufacturing. Most of the existing GDMs [12] add noise separately on the nodes and links in the forward diffusion process while they generate molecules that satisfy a single, eventually large, condition. The proposed GDM variant aims to improve Out-of-Distribution (OOD) [10] for multi-conditioned graph creation tasks. Recent Deep Generative models for topology optimization (TO) proposed in the literature are criticized in terms of both performance and manufacturability. Generative Adversarial Networks as TopologyGAN [13] exploit conditions on physics-based information (i.e., Von Mises stress, strain energy density, and displacement fields) to generate a large number of topologies efficiently but may produce un-manufacturable topologies that violate soft constraints such as volume fraction errors and lead to higher compliance structures. Diffusion Models like TopoDiff [14] proposes a conditional diffusion model, that besides conditioning on fields considers an additional guidance mechanism to encourage the generative process to sample in regions with high manufacturability and high performance. Although it generates samples that satisfy constraints more accurately, TopoDiff is computationally expensive due to iterative sampling, and it not easy to scale to higher dimensionality, complex structures, and 3D domains such as PCMs.
Finaly, Various techniques have been proposed for generating parsimonious subgraphs explaining a given prediction (i.e., property classification, synthetic structure) [16]. As literature on explainable graph methods that are both counterfactual and factual is limited, we will focus on graph perturbation methods allowing us to minimize the complexity of explanations while maintaining their effectiveness by considering not only node and link deletions but also insertion of new ones.

5. Potential Impact

AI4Cooling has the ambition to establish a a self-driving laboratory technology capable of transforming how thermal management components are designed, optimized, and deployed across both commercial and industrial sectors. This is expected to contribute to the Singapore’s strategic focus on digital manufacturing and sustainable technologies. By enabling integrated, AI-accelerated design cycles and reducing prototyping costs, AI4Cooling opens the door to high-performance, locally manufactured thermal management solutions for critical applications, such as data center cooling infrastructure within Singapore’s limited land footprint, high-density power electronics, aerospace systems, and renewable energy systems.

Appendix A. [References]

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