Journal of Applied Physics | EDITORIAL | pubs.aip.org/aip/jap

Machine learning for thermal transport

Cite as: J. Appl. Phys. **136**, 160401 (2024); doi: 10.1063/5.0237818
Submitted: 7 September 2024 · Accepted: 3 October 2024 ·
Published Online: 24 October 2024

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Note: This paper is part of the special topic, Machine Learning for Thermal Transport.
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https://doi.org/10.1063/5.0237818

INTRODUCTION

Heat transfer is a fundamental process that underpins a vast array of applications, from aerospace engineering and power generation to electronics cooling and precision manufacturing. In recent decades, substantial advancements have been achieved in understanding and manipulating thermal transport across various scales, driven by breakthroughs in experimental and simulation techniques. However, significant challenges remain, particularly in addressing complex heat transfer phenomena that span multiple scales and involve multi-physics interactions. These pose challenges to traditional analytical, computational, and experimental methods, underscoring the need for innovative approaches to deepen our understanding and improve our control of thermal transport processes.

Machine learning (ML) has recently emerged as a transformative force in the study of thermal transport.[1–3] Its integration into thermal research is rapidly advancing the study of heat transfer across a wide range of disciplines. With its ability to process vast datasets, discern intricate patterns, and make fast predictions, ML is redefining the boundaries of thermal transport research, particularly in tackling complex problems. This Special Topic is dedicated to showcasing the latest advancements and applications of ML in studying thermal transport, providing a platform for cutting-edge research that pushes the frontiers of this dynamic field.

This Special Topic features 31 papers that explore the application of ML in thermal transport research. The breadth of research demonstrates the versatility and growing importance of ML in this field. These papers are categorized into five main topics: (i) machine learning potentials (MLPs), (ii) predicting thermal properties, (iii) design and optimization, (iv) data analysis, and (v) tutorials, reviews, and perspectives. By leveraging ML, researchers are now able to construct interatomic potentials with *ab initio* accuracy and orders of magnitude improved computational efficiency, predict and optimize thermal properties with unprecedented accuracy, design thermal systems and materials with target performance, and analyze complex datasets from experiments and/or simulations to extract meaningful insights. As the field continues to evolve, the integration of ML is expected to drive further innovation, enabling more efficient energy systems and novel material discoveries that are previously unachievable.

MACHINE LEARNING POTENTIALS FOR THERMAL TRANSPORT

MLPs have emerged as a crucial tool in accurately simulating and predicting thermal transport properties, providing a significant boost in both precision and computational efficiency. Recent progress in the development of these potentials, such as neural network potential,[4] Gaussian approximation potential (GAP),[5] spectral neighbor analysis potential,[6] moment tensor potential (MTP),[7] and neuroevolution potential (NEP),[8] has enabled researchers to tackle increasingly complex systems and phenomena in thermal transport. Yang *et al.*[9] developed a machine-learned atomic cluster expansion (ACE) potential to achieve quantum-accurate thermal simulations for wurtzite aluminum nitride (w-AlN), demonstrating its capability to accurately predict lattice thermal conductivity and other thermal properties, validated against density functional theory (DFT) and experimental results. This potential enabled efficient modeling of thermal behaviors, including the impact of biaxial strains on thermal conductivity and phonon properties, crucial for the design of w-AlN-based electronics. Tang *et al.*[10] developed a neuroevolution potential (NEP) to the transition from 2D to 3D thermal conductivity in hexagonal boron nitride (h-BN), demonstrating that the thermal conductivity decreases rapidly from monolayer to bulk values and saturates beyond four layers due to phonon focusing effects. Similarly, a NEP was constructed by Chen *et al.*[11] to calculate the thermal conductivity of bilayer graphene, h-BN, and their heterostructures, highlighting the significant impact of twist angles on thermal conductivity, with reductions exceeding 35% due to enhanced phonon scattering and anharmonic interactions. Lu *et al.*[12] employed a NEP to investigate the thermal properties of fullerene-encapsulated carbon nanotubes (CNTs), revealing that the presence of fullerene reduces thermal conductivity by approximately 55% compared to empty CNTs, attributed to increased phonon scattering. Liu *et al.*[13] focused on MoS_2/WS_2 heterostructures, developing a deep neural network-based potential to accurately predict mechanical and thermal properties. Their findings showed that the interfacial thermal conductance in these heterostructures is significantly higher than that of graphene-based interfaces, highlighting the potential of their approach for large-scale simulations. In the study of Ga_2O_3 phases, Rybin and Shapeev[14] constructed a MTP to calculate the lattice thermal conductivity of α- and β-Ga_2O_3, highlighting the importance of active learning for generating a robust and accurate interatomic potential while maintaining a moderate-sized training dataset. Similar efforts were devoted to developing a NEP of β- and κ-Ga_2O_3 by Wang *et al.*,[15] revealing notable differences in their thermal conductivities and temperature dependence. Xiang *et al.*[16] used a GAP to explore the impact of high-order scatterings and phonon coherence on hafnia's lattice thermal conductivity, providing new insights into its thermal behavior. Additionally, Yuan *et al.*[17] developed a MTP for Janus XBAlY ($X = Se, S, Te$; $Y = S, Se, O$; $X \neq Y$) monolayers and demonstrated that its thermal conductivity does not always correlate with atomic mass, revealing complex dependencies influenced by phonon scattering mechanisms, bandgaps, and chemical bond strengths. These advances underscore the critical role of MLPs in achieving accurate and efficient simulations, revealing detailed insights into thermal transport phenomena in different materials.

PREDICTING THERMAL PROPERTIES USING MACHINE LEARNING

By leveraging advanced algorithms and integrative frameworks, several articles in this Special Topic showcase the accuracy and efficiency of ML in predicting a wide array of thermal properties, including lattice thermal conductivity, thermal behaviors in disordered structures, interfacial thermal resistance, and heat capacity. Lu *et al.*[18] estimate the lattice thermal conductivity of AlCoCrNiFe high-entropy alloys using a support vector regression model, achieving precise results highlighting the technique's effectiveness in analyzing complex alloy systems. The end-to-end framework developed by Srivastava and Jain[19] integrates data from multiple sources to predict material thermal conductivity, offering a comprehensive solution that enhances predictive accuracy. In the realm of disordered structures, Zhu *et al.*[20] harnessed ML to investigate and manipulate thermal transport in amorphous networks, illustrating the potential of these techniques to optimize materials with intricate thermal behaviors. Deep convolutional neural networks, as applied by Al-Fahdi and Hu,[21] facilitated high-throughput screening for substrate optimization in β-Ga_2O_3, advancing the development of materials with superior interfacial thermal management. Meanwhile, Huang and Barati Farimani[22] employed a multimodal learning strategy based on transformers and crystallography pretraining to predict heat capacity, demonstrating how combining different data modalities can enhance the accuracy and reliability of thermal property predictions. Together, these studies emphasize the transformative impact of ML on thermal property prediction and material science advancements.

DESIGN AND OPTIMIZATION USING MACHINE LEARNING

Another key application of ML is advancing the design and optimization of different engineering systems. A large group of articles report the design and optimization of thermal systems using various ML algorithms, such as the Gaussian process, convolutional neural network, and Bayesian regularization. Chen *et al.*[23] achieved an innovative design of a nonreciprocal thermal absorber, utilizing ML to optimize radiation management in multiple directions and spectral ranges. The development of a nonlinear compact thermal model for GaN high-electron-mobility transistors was realized by Hua *et al.*,[24] who integrated Gaussian process predictors with an ensemble Kalman filter to enhance self-adaptability and predictive accuracy. With a focus on thermal transparency, Liu *et al.*[25] employed a diffusion model-based inverse design approach, achieving precise control over thermal properties. Meanwhile, Luo and Lee[26] advanced thermoelectric cooling techniques through convolutional neural network, addressing the challenge of managing multiple hotspots in thermal systems on demand. Liu *et al.*[27] enhanced the optimization of immersion-cooled battery thermal management systems by integrating ML into co-design strategies, improving overall control and efficiency. In the realm of evaporation, Qiao *et al.*[28] utilized ML algorithms to optimize the evaporation rate in graphene-water systems, leading to more efficient evaporation. Additionally, Vyas *et al.*[29] explored liquid droplet entrainment in annular flow boiling regimes using Bayesian regularization algorithms, demonstrating ML's role in refining complex fluid dynamics models. These contributions highlight the versatility of ML across different applications and have led to innovative solutions in thermal management and system design.

DATA ANALYSIS USING MACHINE LEARNING

ML can also enhance data analysis for experimental thermal measurements and simulations, improving accuracy and efficiency in extracting key thermal properties and parameters from complex and noisy datasets. A deep learning-based method developed by Mao *et al.*[30] enhances the processing of transient thermoreflectance measurements, offering improved accuracy and efficiency. Addressing parameter fitting challenges, Sripada *et al.*[31] applied physics-informed neural networks (PINNs) to robustly extract thermal properties from noisy data acquired through the laser-based Ångstrom method. The BubbleID framework, introduced by Dunlap *et al.*,[32] employs deep learning to analyze bubble interface dynamics, providing new insights into fluid dynamics and heat transfer. In the context of channel flows, Cao *et al.*[33] utilized conditional generative adversarial networks to infer temperature fields from concentration data, presenting a novel approach to thermal field analysis. Rapid subsurface analysis of frequency-domain thermoreflectance images is achieved through K-means clustering, as demonstrated by Jarzembski *et al.*,[34] which enhances the speed and precision of thermal property assessments. Additionally, Ali Boroumand *et al.*[35] employed convolutional neural networks to extract key parameters of 2D natural thermal convection, contributing to a more nuanced understanding of convection processes. Collectively, these advancements demonstrate the power of ML in refining data analysis techniques in heat transfer research and applications.

TUTORIALS, REVIEWS AND PERSPECTIVES

This Special Topic also features a few articles that provide advanced tutorials, comprehensive reviews, and forward-looking perspectives on the integration of ML into thermal transport studies. A mini-review and tutorial by Dong *et al.*[36] surveys the application of MLPs in MD simulations of heat transport and offers a detailed implementation on how to develop a NEP and utilize it to model heat transport within the GPUMD framework. In another tutorial, Huang and Ju[37] introduce the fundamentals and implementation of a machine-learning-assisted method for the active design of polymers with high intrinsic thermal conductivity, illustrating how artificial intelligence can be harnessed to optimize polymer materials. The review by Hu *et al.*[38] surveys the use of ML in identifying thermally conductive polymers, highlighting significant advancements and methodologies in this field. Additionally, Hu[39] provides a comprehensive perspective on the challenges and future directions for applying artificial intelligence to thermal transport, emphasizing the transformative potential of artificial intelligence in this area. Together, the educational tutorials, reviews, and perspectives included in this Special Topic provide critical literature survey and perspective, enabling researchers to incorporate ML techniques into their own work, thus broadening the impact of ML in thermal transport research.

CONCLUSION

This Special Topic underscores the profound impact of ML on thermal transport research and offers a valuable resource for both experienced researchers and newcomers. The contributions within this issue illustrate how ML is transforming both the fundamental understanding and practical applications in the field. By integrating ML techniques into various aspects of thermal transport, researchers are pushing the boundaries of atomistic simulation, property prediction, material design, and data analysis.

However, despite the encouraging advancements of ML in thermal transport research, significant challenges remain that must be addressed to fully realize its potential. A key limitation is the transferability of ML models, which often struggle to generalize beyond the specific material systems or conditions they were trained on, necessitating extensive retraining for new scenarios. Additionally, the scarcity of high-quality training data presents a substantial barrier, as it is often challenging to find adequate data for training, and the complexity and variability of thermal properties further complicate the creation of comprehensive datasets, potentially resulting in models that lack accuracy or robustness. Furthermore, the interpretability of ML models remains a critical concern, as the black-box nature of many algorithms can obscure the physical insights they capture, potentially reducing trust in their predictions and hindering broader adoption in practical applications. Overcoming these challenges is essential for advancing the application of ML and unlocking its full potential.

Looking ahead, the integration of ML into thermal transport research holds the promise of driving significant advancements. As ML techniques continue to evolve and extend into new research areas, they are poised to further advance the study of thermal transport. We hope that the findings and discussions presented will inspire continued exploration and innovation, ultimately leading to breakthroughs that will benefit thermal science and engineering.

ACKNOWLEDGMENTS

We thank all authors who contributed to this Special Topic. Special thanks go to the staff at the AIP Publishing, especially Dr. Jessica Trudeau, Dr. Jaimee-Ian Rodriguez, and Dr. Brian Solis for their assistance in preparing this Special Topic. We are also grateful to all the editors and reviewers for their outstanding commitment and contributions to this Special Topic. R.G. acknowledges the support from the Excellent Young Scientists Fund (Overseas) of Shandong Province (Grant No. 2022HWYQ-091), the Taishan Scholars Program of Shandong Province (Grant No. tsqnz20221163), the Natural Science Foundation of Shandong Province (Grant No. ZR2022MA011), and the Initiative Research Fund of Shandong Institute of Advanced Technology. A.M. acknowledges the support from Army Research Office under Award No. W911NF2220191.

AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Ruiqiang Guo: Writing – original draft (lead); Writing – review & editing (lead). **Bing-Yang Cao:** Writing – review & editing (equal). **Tengfei Luo:** Writing – review & editing (equal). **Alan J. H. McGaughey:** Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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