Differentiable Phonon Hydrodynamic Simulations for Inverse Design and Material Property Extraction

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The geometry of a nanostructure strongly influences its transport properties, including its effective thermal conductivity. Nondiffusive phenomena—such as hydrodynamic transport—introduce novel mechanisms for tuning heat flow beyond what is captured by Fourier's law. However, engineering nanostructures for thermal applications remains challenging due to computational complexity. Most existing efforts rely on trial-and-error approaches or gradient-free methods, such as genetic algorithms, which suffer from slow convergence and poor scalability. In this talk, I will present our recent work on geometry optimization via differentiable programming. Our approach leverages automatic differentiation to compute gradients of a cost function with respect to the material's geometry, described through a density field. This enables efficient gradient-based optimization. We combine density-based topology optimization with the mode-resolved phonon Boltzmann transport equation (BTE) to design materials with a target effective thermal conductivity tensor. Our topology optimization approach is based on the *Transmission Interpolation Method* (TIM) [1], a novel scheme that connects material density to interfacial heat flux. In the second part of the talk, I will show how our differentiable BTE solver can be integrated with experimental data to extract key thermal properties. I will also highlight emerging directions at the intersection of thermal transport and differentiable programming, such as inverse-designed structures for analog computing [2]. The talk will conclude with an overview of the open-source software supporting our work.

[1] G. Romano, and S. G. Johnson. "Inverse design in nanoscale heat transport via interpolating interfacial phonon transmission." Structural and Multidisciplinary Optimization 65.10 (2022): 297.

[2] S. Caio and G. Romano. "Analog Computing with Heat: Matrix-vector Multiplication with Inverse-designed Metastructures." arXiv preprint arXiv:2503.22603 (2025).