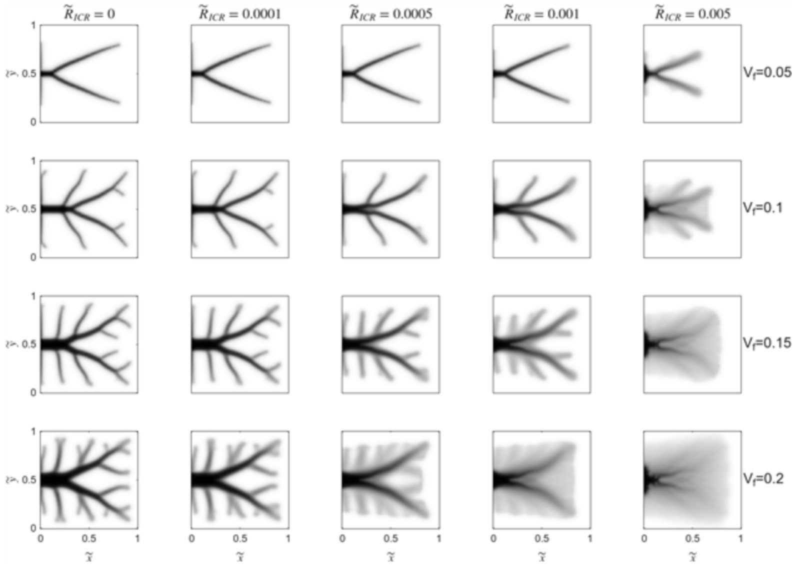
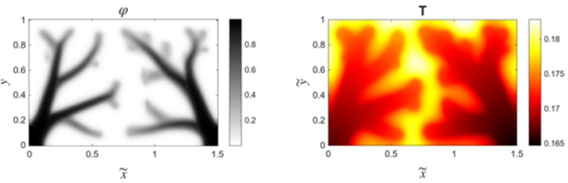
Emergence of Constructal Thermal Networks: Topology Optimization with Rigorous Kapitza Interfacial Calculus

Yoav Tsori[1]

[1]Ben-gurion University Of The Negev, Beer Sheva, Israel



The macroscopic transport properties of multi-phase composites and soft-matter systems are fundamentally governed by microscopic interfacial boundary conditions. In conductive networks, the Kapitza contact resistance at the boundaries of highly conductive inclusions frequently dictates the global limits of energy dissipation. Standard computational design methods, which largely rely on isotropic material interpolation, inherently fail to capture this severe, highly directional interfacial resistance, either vastly over-predicting effective conductivities or relying on computationally fragile explicit interface-tracking algorithms. To bridge this gap, we present a rigorous computational framework to predict the emergence of optimal heat-routing architectures in systems dominated by severe interfacial thermal resistance.



Utilizing a phase-field-like continuous density representation coupled with a Helmholtz partial differential equation (PDE) filter, we derive an exact continuous sensitivity calculus via integration by parts. Instead of relying on artificial geometric penalties, the interfacial physics are embedded directly into the governing heat equation. We define a covariant thermal resistivity tensor as the sum of an isotropic bulk resistivity and an anisotropic boundary penalty: $\rho(\tilde{\phi}) = \rho_{\text{bulk}}\mathbf{I} + \tilde{R}_{\text{ICR}}\,|\nabla\tilde{\phi}|\,(\mathbf{m}\otimes\mathbf{m})$. This formulation natively captures the Kapitza resistance along dynamically evolving phase boundaries without requiring explicit interface tracking, strictly penalizing the normal component of heat flux while leaving tangential conduction unimpeded. By mathematically neutralizing spurious boundary heat leaks and enforcing strict thermodynamic M-matrix conditions, our stabilized adjoint-based solver suppresses unphysical checkerboard artifacts and resolves thermodynamically pure structures.

Applying this continuous mathematical engine to domains with localized high-flux thermal gradients, we demonstrate that interfacial resistance drives a striking macroscopic morphological phase transition. Without a Kapitza penalty, the solver minimizes bulk transport distance by generating standard, infinitely branching, capillary-like dendritic networks. However, as the physical interfacial penalty increases, the thermodynamic cost of maintaining a massive diffuse surface area overwhelms the volumetric conduction benefit. The algorithm organically forces a topological shift, heavily penalizing the fine capillary networks and giving way to the emergence of thickened, fully connected constructal Bejan trees governed by a physical Kapitza length scale.

These findings provide a rigorous, bounded thermodynamic basis for understanding optimal transport geometries in complex multiphase systems. By natively capturing the physical limits of microscopic heat transfer, this method offers a predictive computational tool for the fundamental design of advanced thermal metamaterials, microelectronic cooling networks, and highly loaded polymer composites.