Inverse Design in Nanoscale Devices

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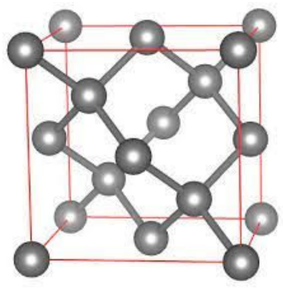
We propose the development of a differentiable physics solver to compute and optimize nanoscale electronic transport. This tool will enable constrained large-scale device optimization, opening up opportunities for novel computing architectures and end-to-end concurrent software and hardware optimization.

Optimization Framework



Objective function
- High electrical conductivity
- Low leakage current
- Low thermal conductivity

Constraints
- High mechanical stability
- Maximum volume
- Geometry constraints
- …

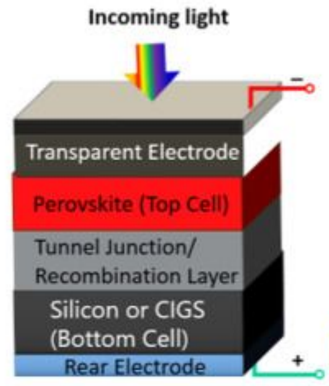
Geometry (**ρ**)

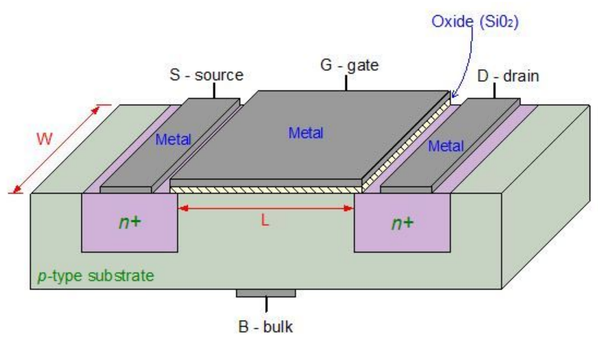
Input

Forward/Adjoint BTE solver

Objective function g(**ρ**) vector-Jacobian-product vJp(**v**)

Optimized device





OpenBTE

G. Romano, https://arxiv.org/abs/2106.02764

Electron-Phonon Boltzmann Transport Equation

Electron population — Electromagnetic force — External excitation

$$\frac{\partial f_n(\mathbf{r},\mathbf{k},t)}{\partial t} + \mathbf{v}_n(\mathbf{k})\cdot\nabla f_n(\mathbf{r},\mathbf{k},t) + \mathbf{F}(\mathbf{r},t)\cdot\nabla_{\mathbf{k}} f_n(\mathbf{x},\mathbf{k},t) = C_n^{\mathrm{el}}\{f,n\} + Q(\mathbf{r}) \quad \textbf{(electrons)}$$

Electron velocity — Electron Scattering Operator

Phonon population

$$\frac{\partial n_s(\mathbf{r},\mathbf{q},t)}{\partial t} + \mathbf{v}_s(\mathbf{q})\cdot\nabla n_s(\mathbf{r},\mathbf{q},t) = C_s^{\mathrm{ph}}\{f,n\} \quad \textbf{(phonons)}$$

Phonon velocity — Phonon Scattering Operator

Electrostatic potential

$$-\nabla\cdot[\epsilon(\mathbf{r})\nabla\varphi(\mathbf{r})] = \rho(\mathbf{r})$$

Dielectric constant — Total charge

Electric field

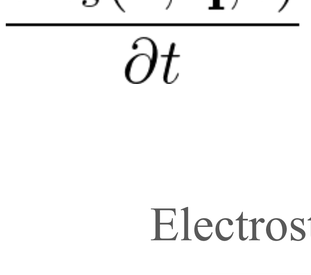
$$\mathbf{F}_n(\mathbf{r}) = -\frac{e}{\hbar}\left[\mathbf{E}(\mathbf{r}) + \mathbf{v}_n(\mathbf{k})\otimes\mathbf{B}(\mathbf{r})\right]$$

Magnetic field

Discretization

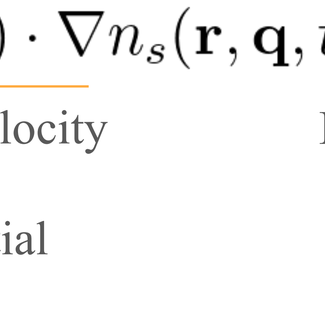
Reciprocal space

$\mathbf{k},\mathbf{q}$:

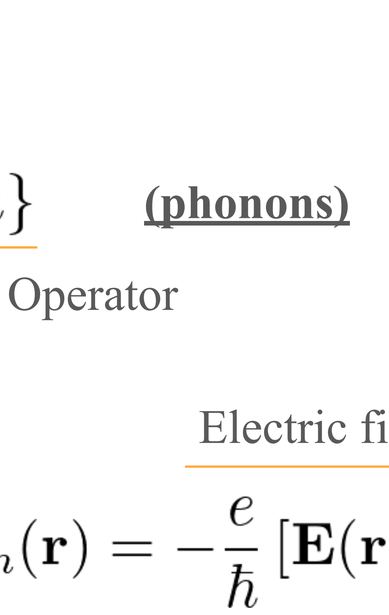


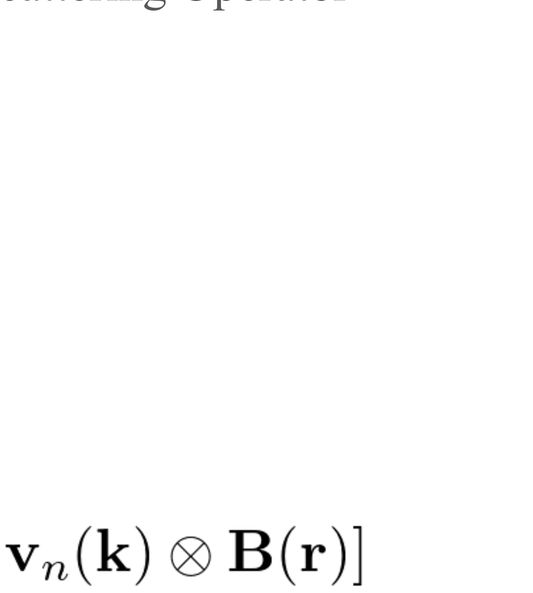
Real space

$\mathbf{r}$:



Optimized Thermoelectric Materials





Giuseppe Romano and Steven G. Johnson. "Inverse design in nanoscale heat transport via interpolating interfacial phonon transmission." Structural and Multidisciplinary Optimization 65.10 (2022): 297.

Acknowledgments

MIT-IBM Watson AI Lab
NASA JPL
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MITei MIT Energy Initiative