ME 697R: Computational Methods for Nanoscale Energy Transport

Chapter 8: Machine learning techniques in nanoscale energy transport
Section 8.3: Machine learning based nanostructure optimization

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Thermoelectric Applications

- Thermoelectric cooling or power generation:
  - Temperature gradient needs to be maintained across the hot and cold junctions.

- Performance characterization: \[ ZT = \frac{S^2 \sigma T}{k_e + k_{ph}} \]

- Low lattice thermal conductivity gives high performance.
Increasing phonon scattering produces low thermal conductivity.

Introducing interfaces within the structure increases phonon scattering:
- Superlattice (SL) is a system with periodic interfaces.
- Phonon scatters at an interface.
- Scattering increases with more interfaces.
- Introducing many periodic interfaces cannot lower thermal conductivity further since some phonons pass through the interface.
- Long wavelength phonons pass through the interfaces without scattering.
Aperiodic Superlattices (Random Multilayers)

- These phonons in periodic superlattices can be scattered by randomizing the layer thicknesses.

- We want to find the random multilayer (RML) structure with lowest thermal conductivity.
Genetic Algorithm

- Optimization of multilayer structures for low (or high) thermal conductivity
  - The problem statement: In a multilayer system with N layers, where each layer can be Material A or B, which structure has lowest thermal conductivity?
    
    Note: For $N=40$, number of possible designs = 30 billion!
  
  - The solution method: Genetic Algorithm based optimization

Natural Selection in action

Crossover and mutation
Principles of Genetic Algorithm:

- **Iterative process**: A group of solutions (called “population”) is evaluated at each iteration.
- **Natural selection**: After each iteration, only the best solutions of the “population” are carried forward and rest are discarded.
- **Evolutionary operators**: Using best solutions of the “population” in $n^{th}$ iteration, selection, crossover and mutation are done to obtain the $(n+1)^{th}$ population.

**Selection**: Probability of selection $\propto$ Fitness of solution
Flow Chart

Initialization of population

Evaluation of fitness of each member using NEMD simulations

Is change in $\kappa$ below tolerance?

YES

Optimized structures achieved

NO

Selection, crossover and mutation

Crossover

Mutation

Roy Chowdhury et al. Nano Energy 2019, under review
GA Optimization Results

- Several independent runs performed, with different starting conditions and different implementations of operators.

- The above run was started from the entire population having worst possible structure, and still our GA was able to find the best structure!

Roy Chowdhury et al. Nano Energy 2019, under review
Understanding the Physics

- Uncovering new physics from optimized structures

Roy Chowdhury et al. Nano Energy 2019, under review
Neural Network

- **Optimization of multilayer structures for low (or high) thermal conductivity**
  - **The problem statement**: In a multilayer system with $N$ layers, where each layer can be Material A or B, which structure has lowest thermal conductivity?

(Same as previous case study)

- **The solution method**: Neural network enabled optimization

- The most computationally expensive step is the MD simulation of the structure.

- We can replace the expensive MD simulation with very fast Neural Network evaluation of $k$ from input structure
**Neural Network**

- **Neural network**: Algorithms inspired by the biological brain functions, that can learn from a large set of examples.

  - The “**architecture**” of the network (# of layers, # of neurons in each layer, activation functions) need to be carefully chosen.

  - The weights of the connections are fitted by “**training**” the network to large number of MD simulated data points.

![Diagram of a neural network](image)

- Input the descriptors of the RML
  - Input layer
  - Hidden layer 1
  - Hidden layer 2
  - Output layer

- Thermal conductivity as output

- W/m-K: 2.3
Convergence during training is monitored by validating NN results over another independent set called “testing set”

2 layer NN, 2000 (L1) + 10 (L2) neurons, ~1200 training set (20 UC)

NN is able to capture the physics!