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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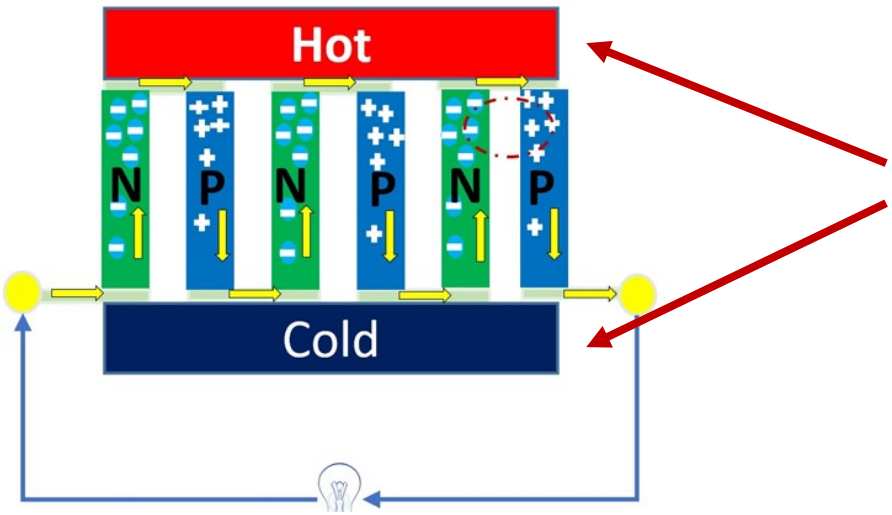
Thermoelectric Applications

- Thermoelectric cooling or power generation:



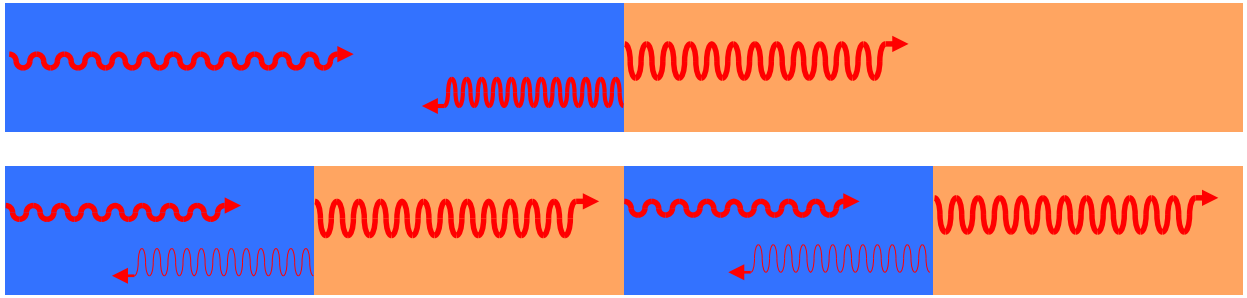
Temperature gradient needs to be maintained across the hot and cold junctions

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

- Low lattice thermal conductivity gives high performance

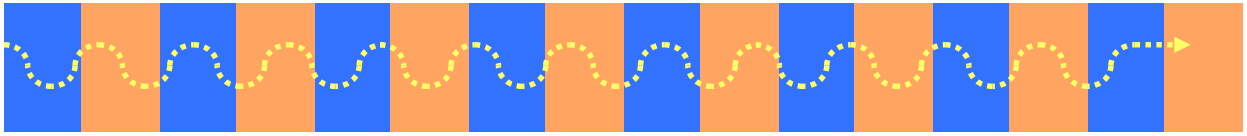
Interfaces and Superlattices

- 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

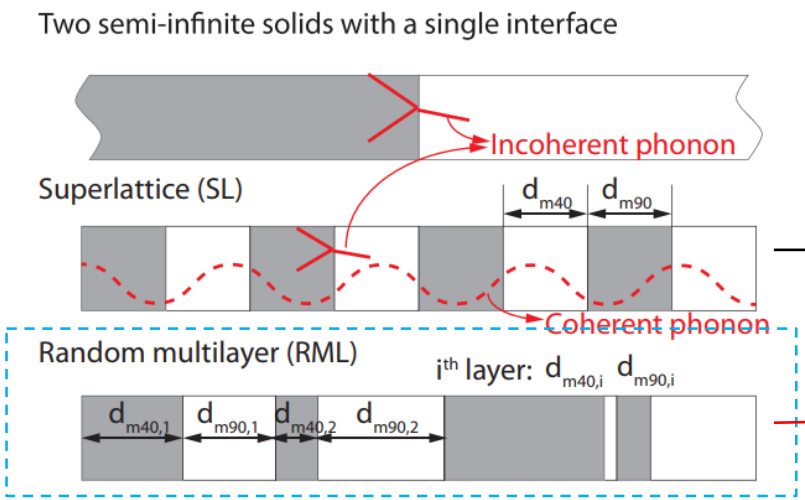


Superlattice

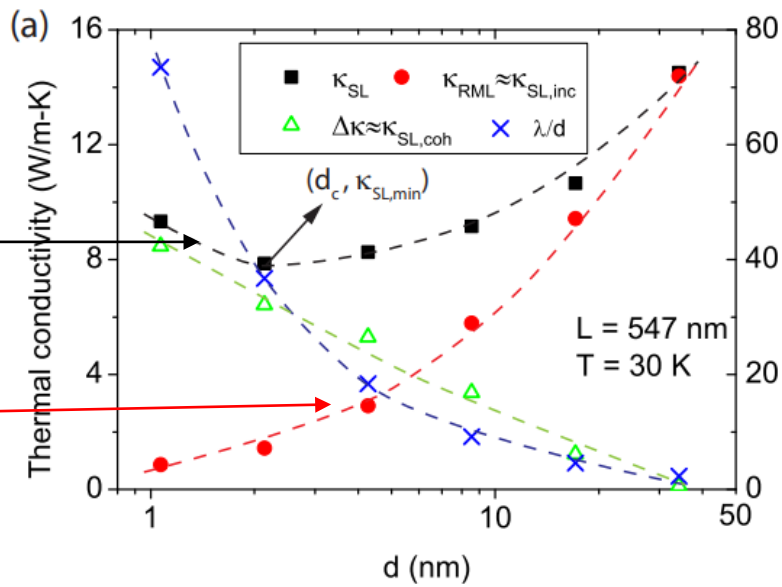
- Long wavelength phonons pass through the interfaces without scattering

Aperiodic Superlattices (Random Multilayers)

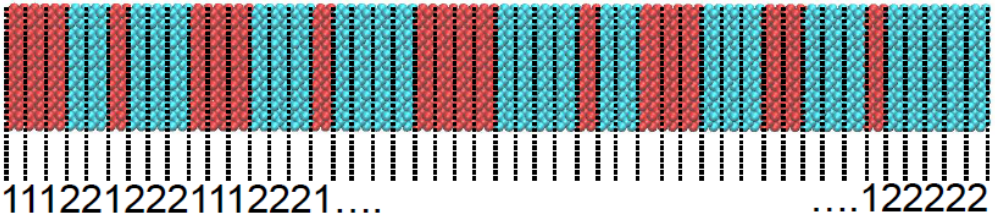
- These phonons in periodic superlattices can be scattered by randomizing the layer thicknesses



Wang *et al.* PRB **90**, 165406 (2014)c

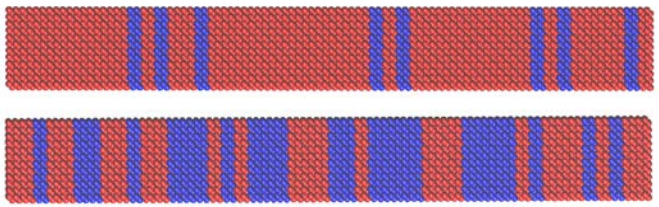


- We want to find the random multilayer (RML) structure with lowest thermal conductivity



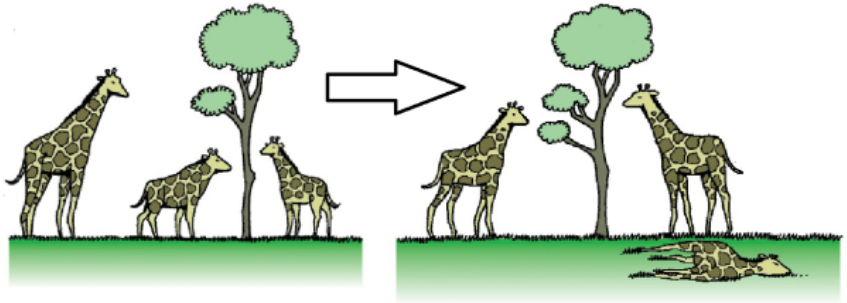
Genetic Algorithm

- **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?

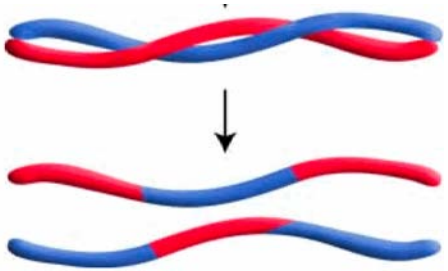


Note: For **N=40**, number of possible designs = 30 billion!

  - The solution method: **Genetic Algorithm** based optimization



Natural Selection in action



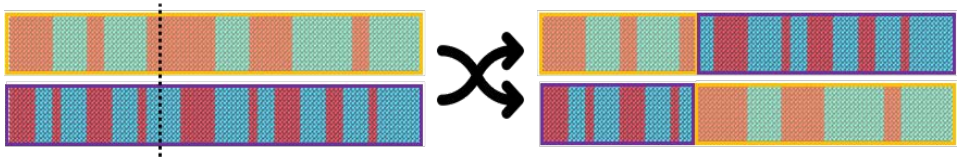
Crossover and mutation

Genetic Algorithm

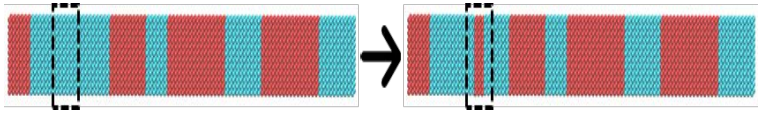
- Principles of Genetic Algorithm:
  - Iterative process: A group of solutions (called "population") is evaluated at each iteration.
  - Natural selection: After each iteration, only the best solutions of the "population" are carried forward and rest are discarded.
  - Evolutionary operators: Using best 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 ∝ Fitness of solution

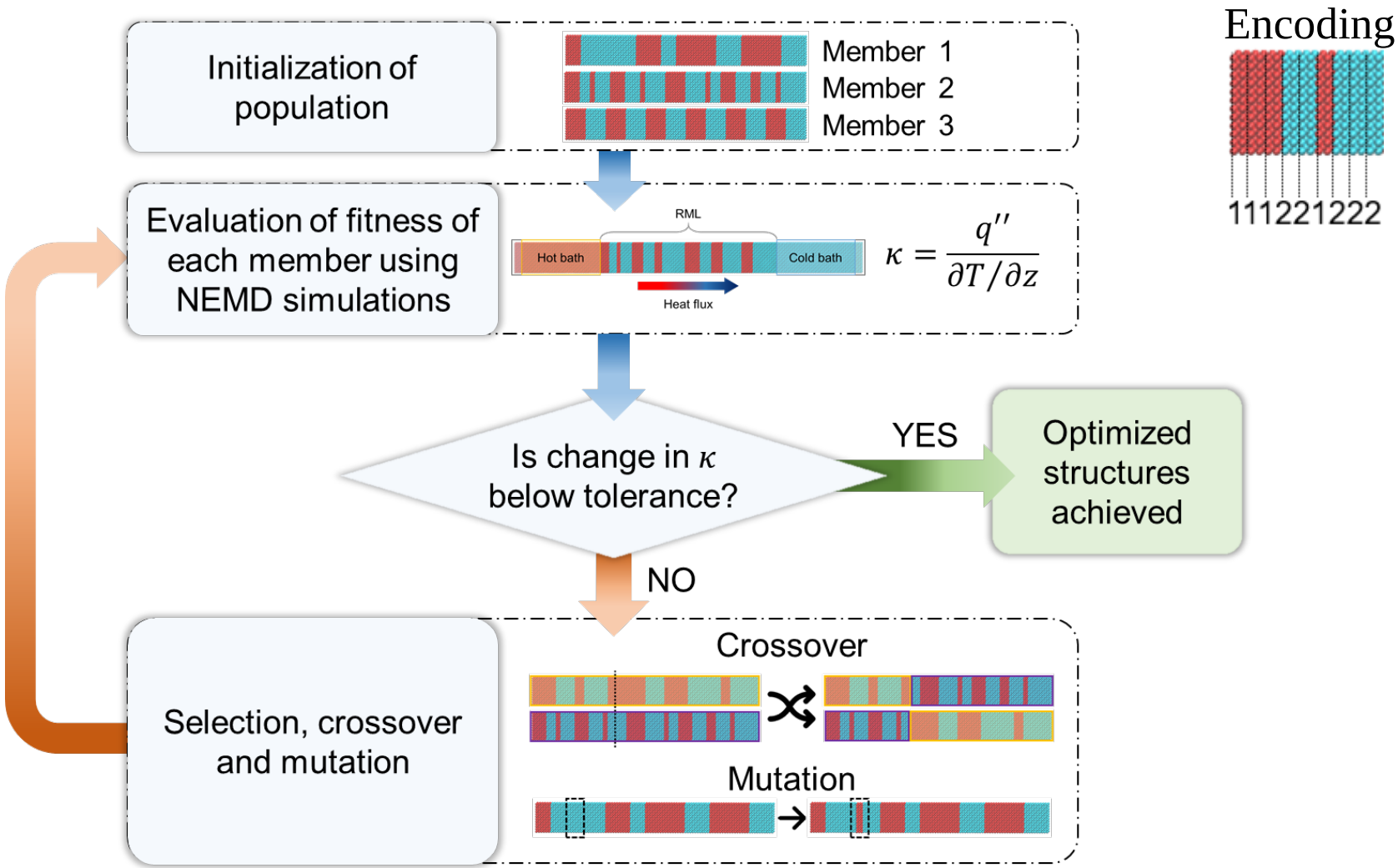
Crossover



Mutation



Flow Chart



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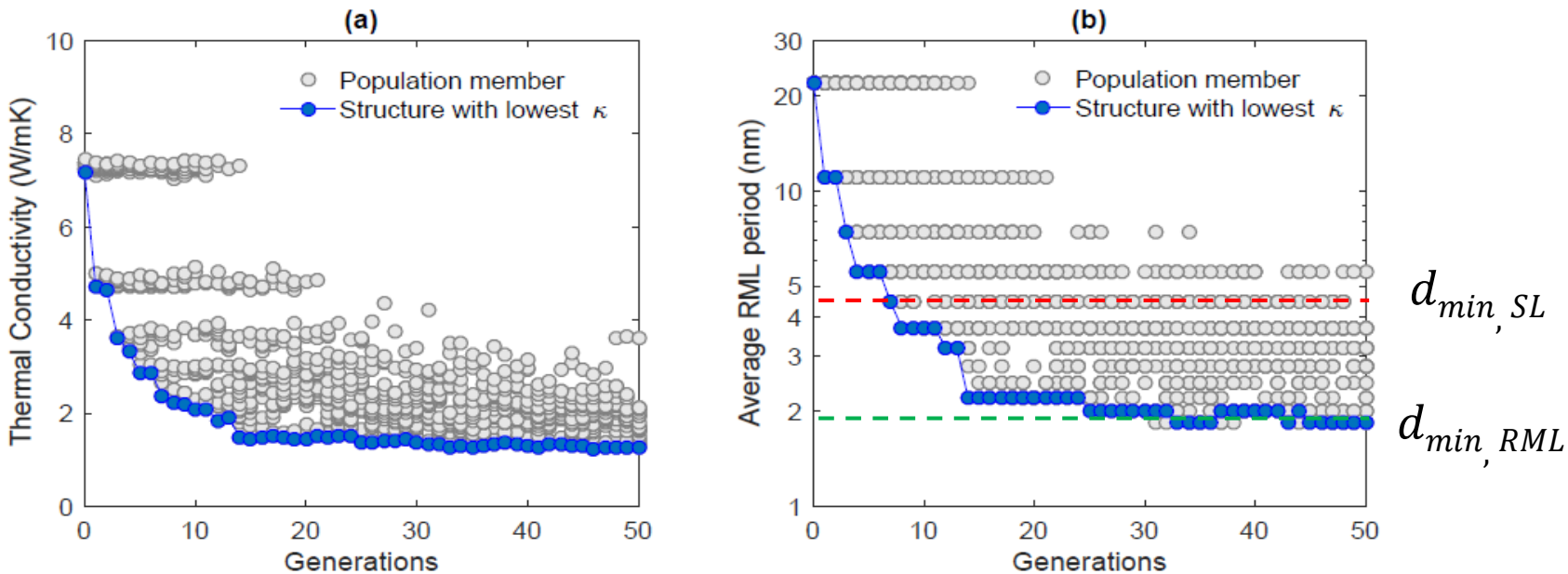
GA Optimization Results

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



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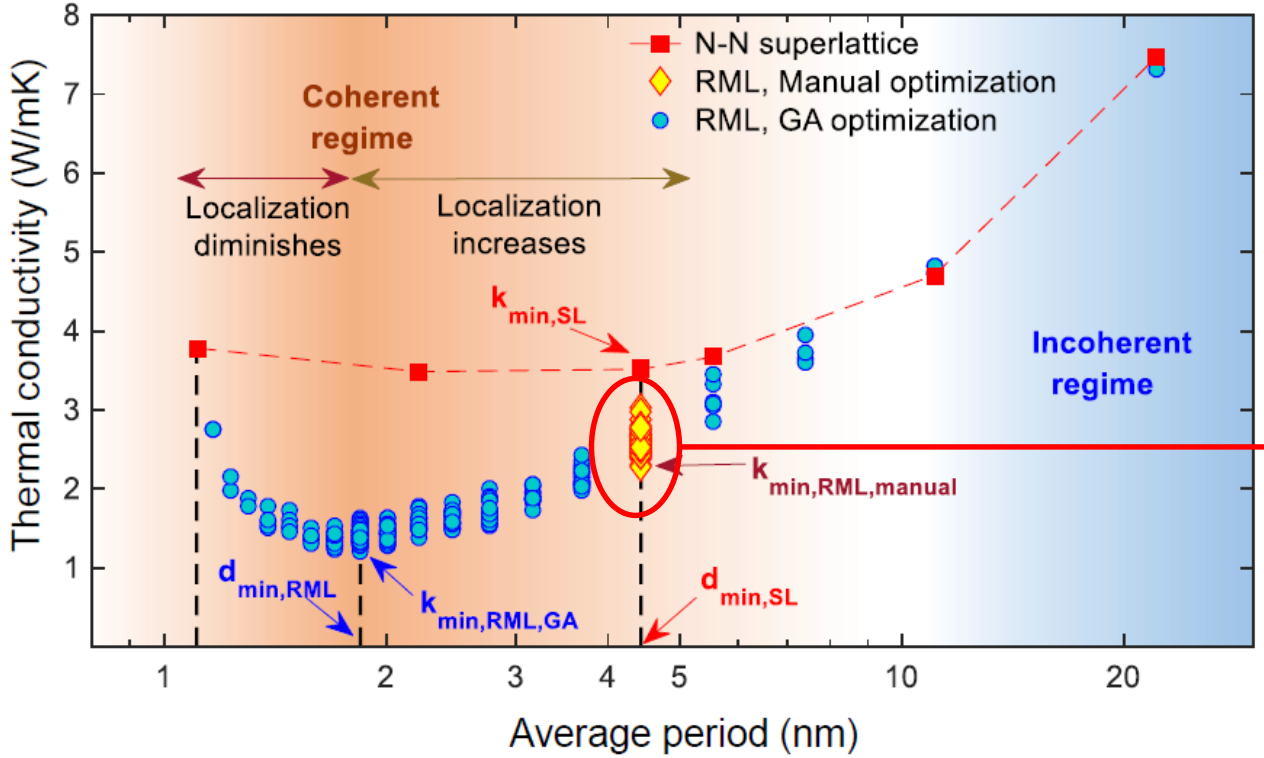
- The above run was started from the entire population having worst possible structure, and still our GA was able to find the best structure!

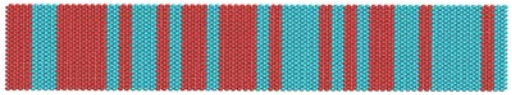
Understanding the Physics

- Uncovering new physics from optimized structures

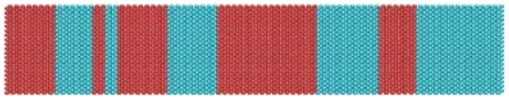


Manual search converges to local minimum

Reduced scope of randomization



Optimized structure



Low incoherent scattering

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Neural Network

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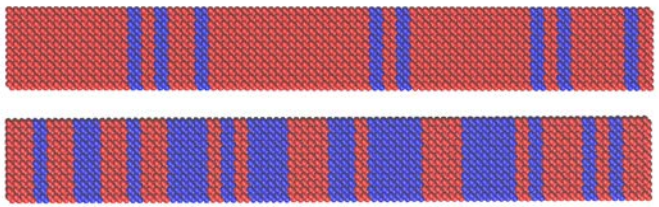


(Same as previous case study)

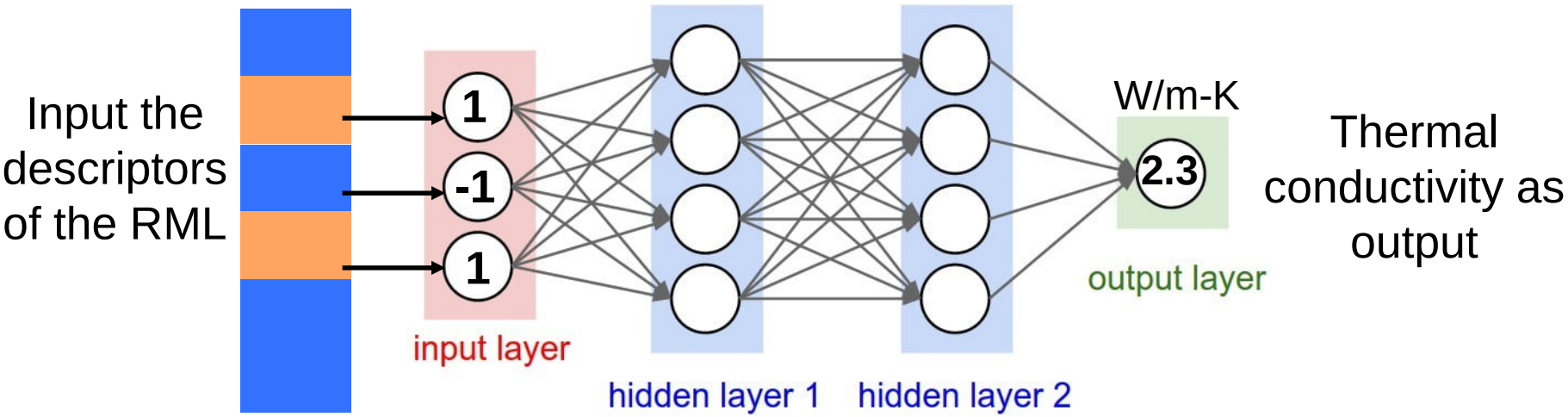
- The solution method: **Neural network** enabled optimization

- 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

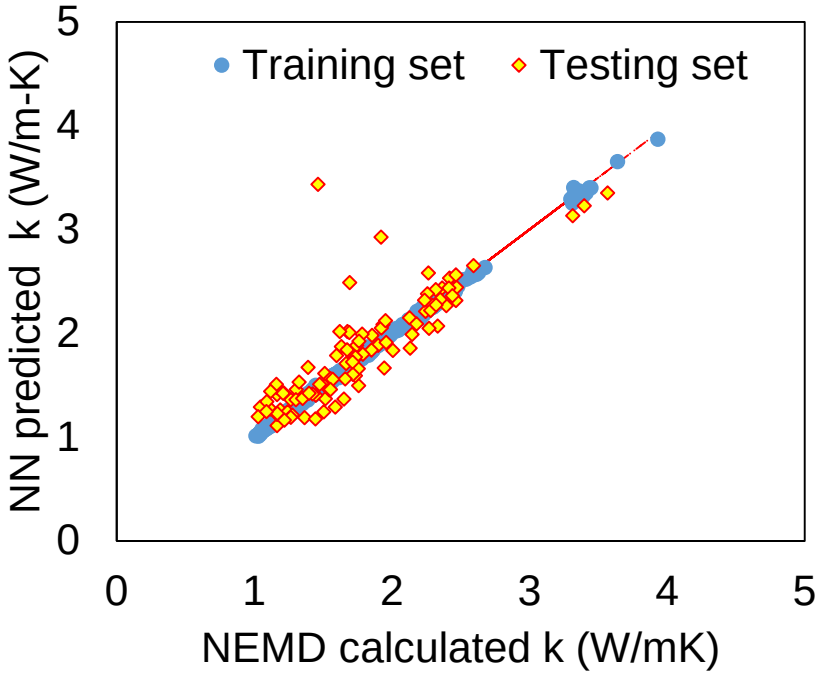


- The "architecture" of the network (# of layers, # of neurons in each layer, activation functions) need to be carefully chosen

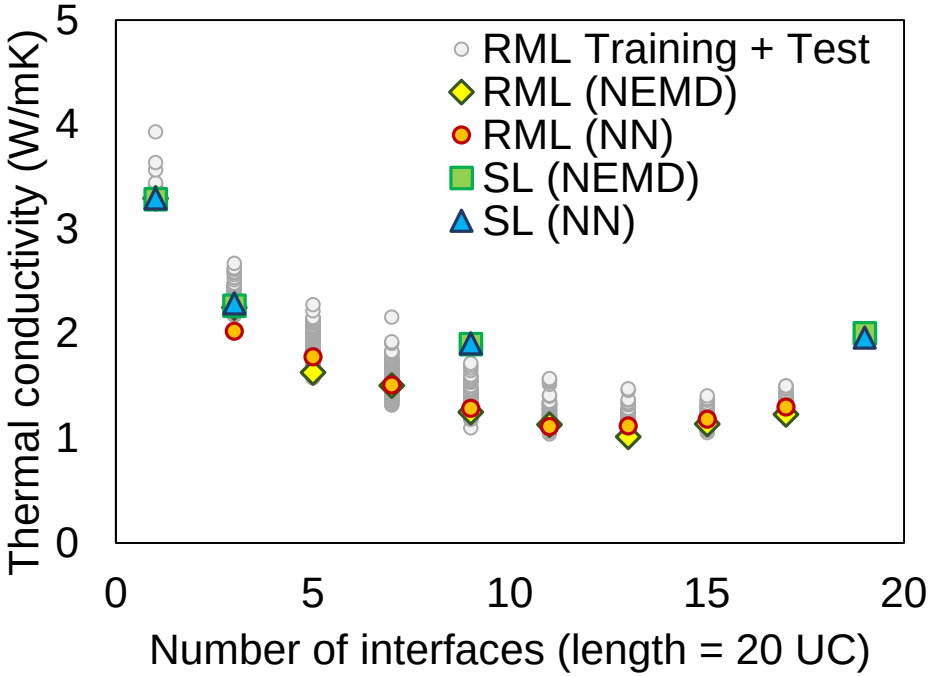
- The weights of the connections are fitted by "training" the network to large number of MD simulated data points

Training and Testing Sets

- 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!