

Objective:

- Understand transport with incoherent scattering – energy and phase loss

Requirements:

- Realistic device extensions
- Atomistic basis
- General phonon description

Approach:

- NEGF problem formulation
- Tight binding basis
- Consider nanowires first
- All phonon modes, free wire
- Multi-Level parallelism (V,E,space)

Computational Burden:

- 70,000 cores for 12 hours
=> ~96CPU years!

Impact:

- first atomistic/incoherent sims
- Model potential drop in emitter

