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A First Principles Approach to Spectral Phonon Transport in Heterostructures

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Changing the World's Energy Future

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Idaho National Laboratory

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A first principles approach to spectral phonon transport in heterostructures

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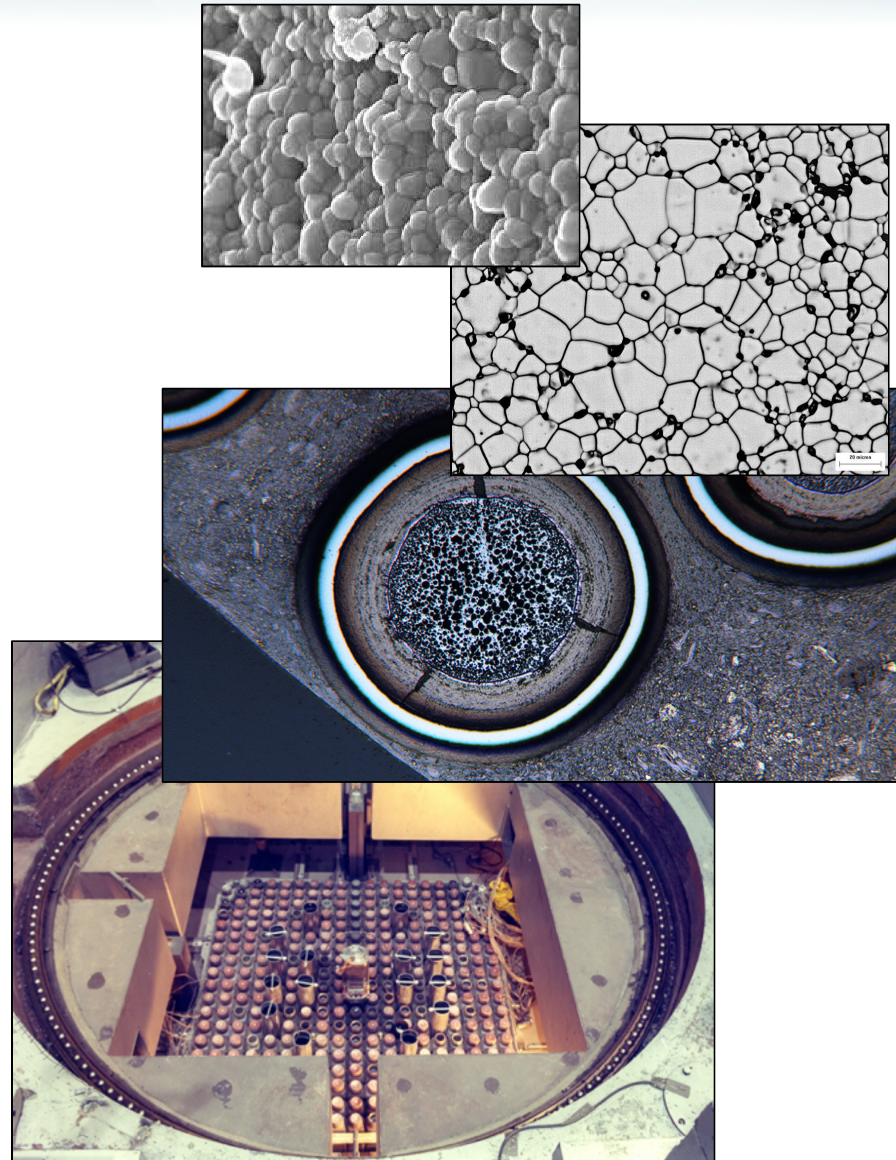
Outline

- Motivation and applications of microscale heat transport
- Material property generation
- Derivation of thermal interface resistance equations
- Results
- Conclusions

Motivation

Thermal properties

- Insights on thermal properties are critical to understanding thermal performance



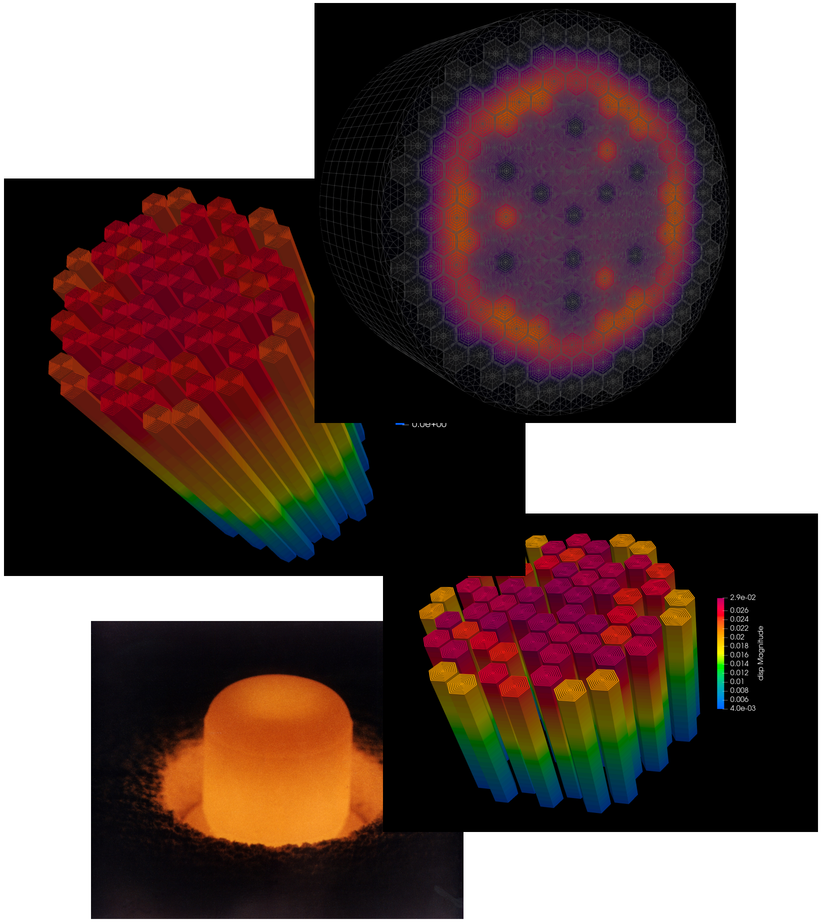
- But these *macroscopic* quantities used in engineering applications are affected by changes at the *microstructural* and *atomic* level

Motivation

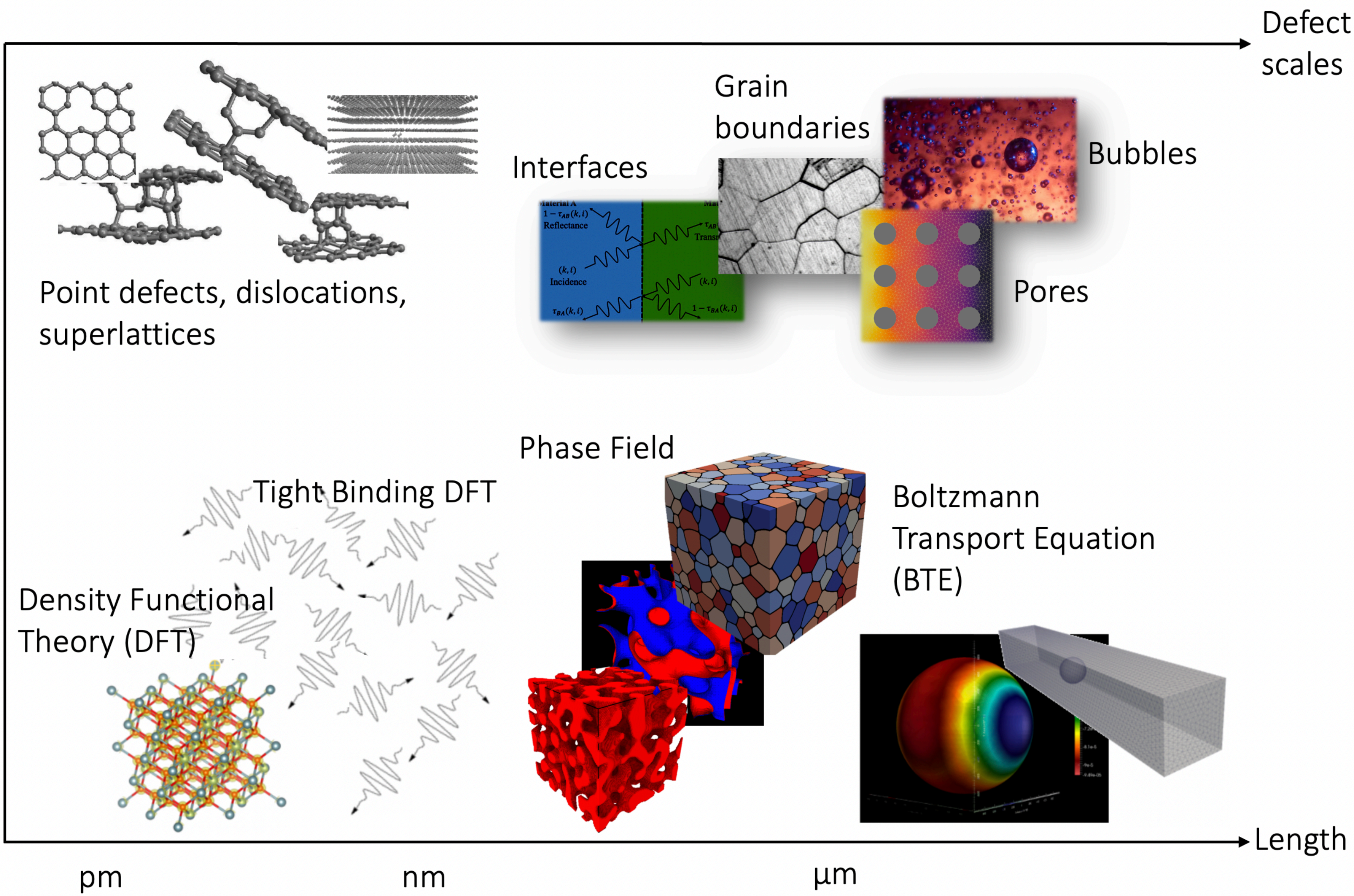
Nuclear reactor fuel performance

MOOSE

- Predicting fuel performance and reactor control is mission critical for Gen-IV technologies
  - UO_2, U_3Si_2, UC, UPuZr
  - Ceramic, metallic, or hybrid
- Neutron cross sections and fuel performance categorically different based on
  - Fuel material
  - Neutron spectrum
  - Burnup
- What do we want? Safe nuclear power, efficient reactors
  - Accident tolerance
  - Robust fuel material



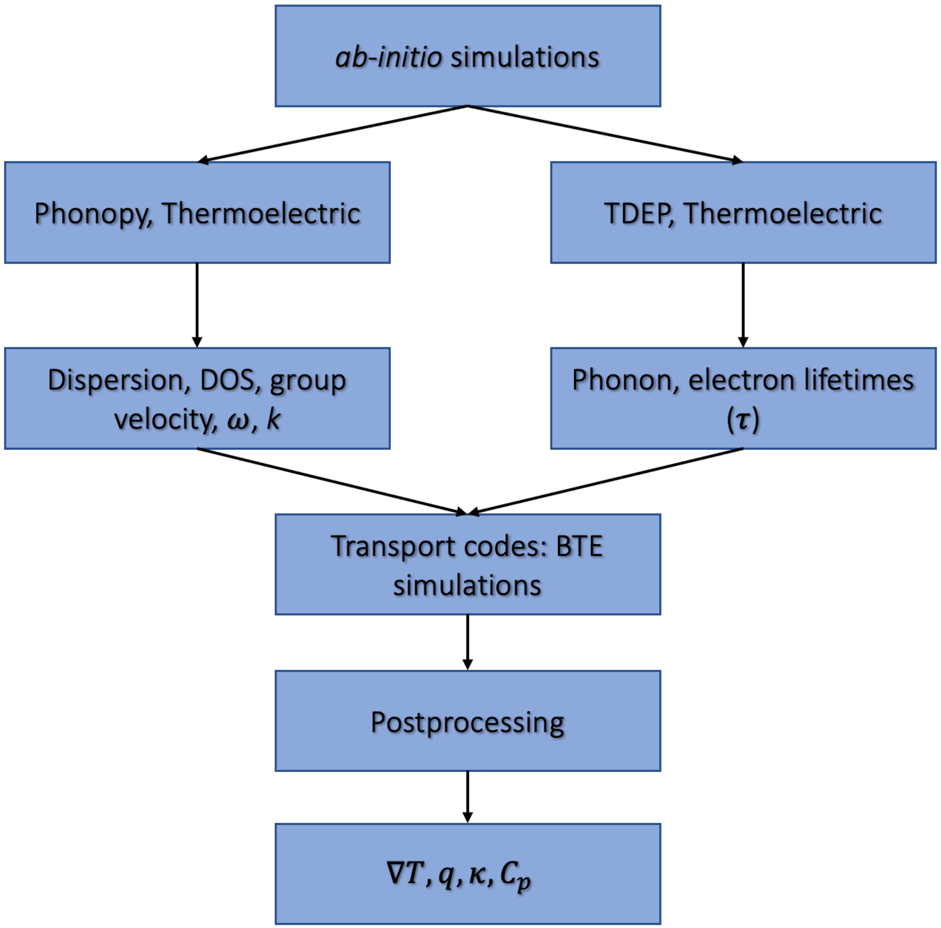
Scale and defect regimes in heat transport



Heat transport workflow

Material property generation

- *ab-initio* simulations
  - Phonon/electron dispersion
  - Density of states
  - Relaxation times
- Material properties into transport codes
- BTE simulations
- Results: heat flux, thermal conductivity, temperature distributions, heat capacity
  - Stop here or pass values to other codes in multiphysics simulation
- Preprocessing, postprocessing



Thermal interfacial resistance

Spectral phonon BTE

- Phonon transport equation in self-adjoint angular flux (SAAF) form

$$-\hat{\mathbf{\Omega}} \cdot \nabla \left[\Lambda \hat{\mathbf{\Omega}} \cdot \nabla \psi \right] + \frac{1}{\Lambda}\psi = \frac{1}{4\pi} \left[\frac{\phi^0}{\Lambda} - \hat{\mathbf{\Omega}} \cdot \nabla \phi^0 - \frac{\beta \phi^0}{|\mathbf{v}|} + \hat{\mathbf{\Omega}} \cdot \nabla \frac{\Lambda \beta \phi^0}{|\mathbf{v}|} \right]$$

  - is measure of the balance of the equilibrium phonon population against the transport system population

- Temper... d with ... r
  phonon ... a func

$$\phi_g^{\mathrm{T}} = \sum_{m=1}^{M} \psi_{m,g} w_m$$

$$\phi^0 = \phi^0 \left(T(\mathbf{r}), \hat{\mathbf{\Omega}}, \xi, p \right) = \frac{\hbar\omega \, \mathbf{v} \, \mathbb{D} d\eta}{\exp\left[\frac{\hbar\omega}{k_B T(\mathbf{r})} \right] - 1}$$

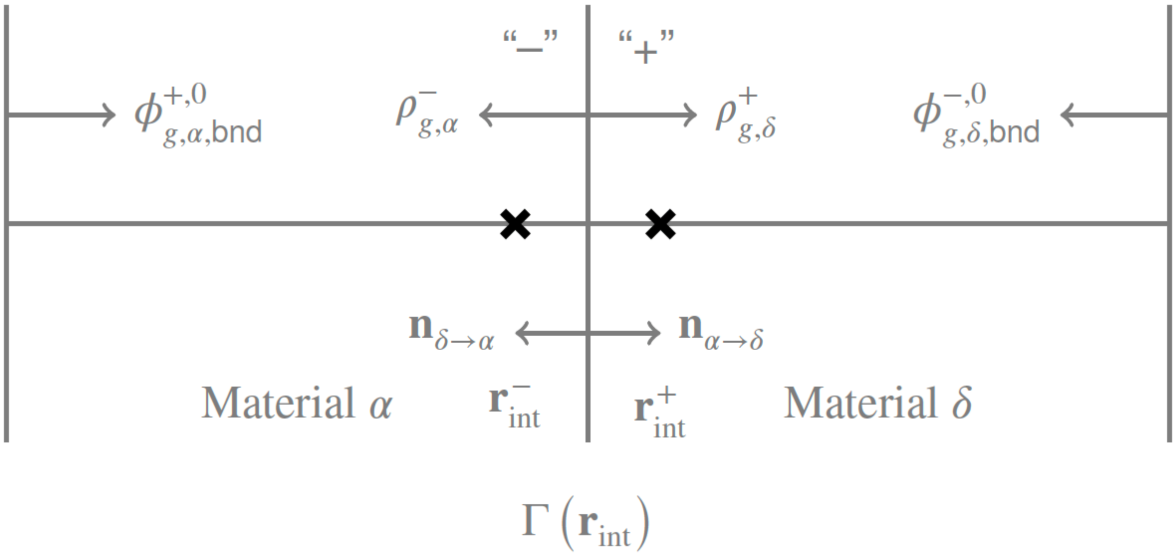
$$T_g(\mathbf{r}) = \frac{1}{k_B} \frac{\hbar\omega_g}{\ln\left[\frac{\hbar\omega_g v_g \mathbb{D}_g}{\phi_g^{\mathrm{T}}(\mathbf{r})} + 1 \right]}$$

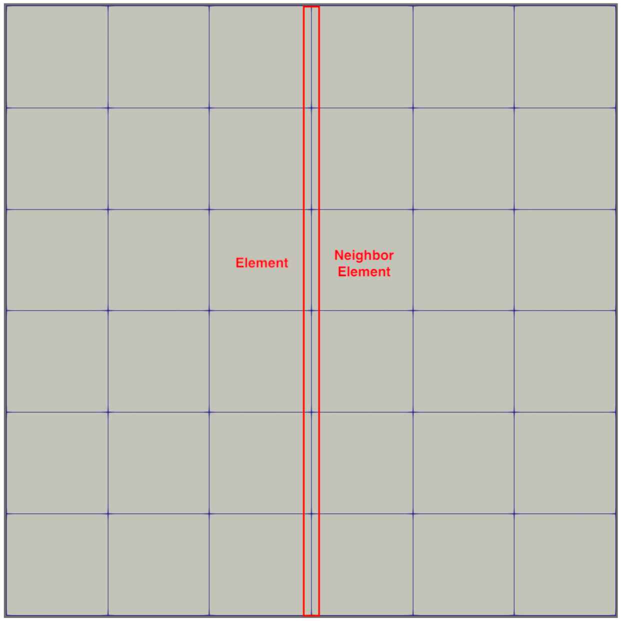
$$C_g = \mathbb{D}_g \omega_g \hbar \frac{\partial n\left(\omega_g, T_g\right)}{\partial T}$$

$$T(\mathbf{r}) = \frac{\sum_{g=1}^{G} C_g T_g}{\sum_{g=1}^{G} C_g}$$

Thermal interfacial resistance

Interface physics



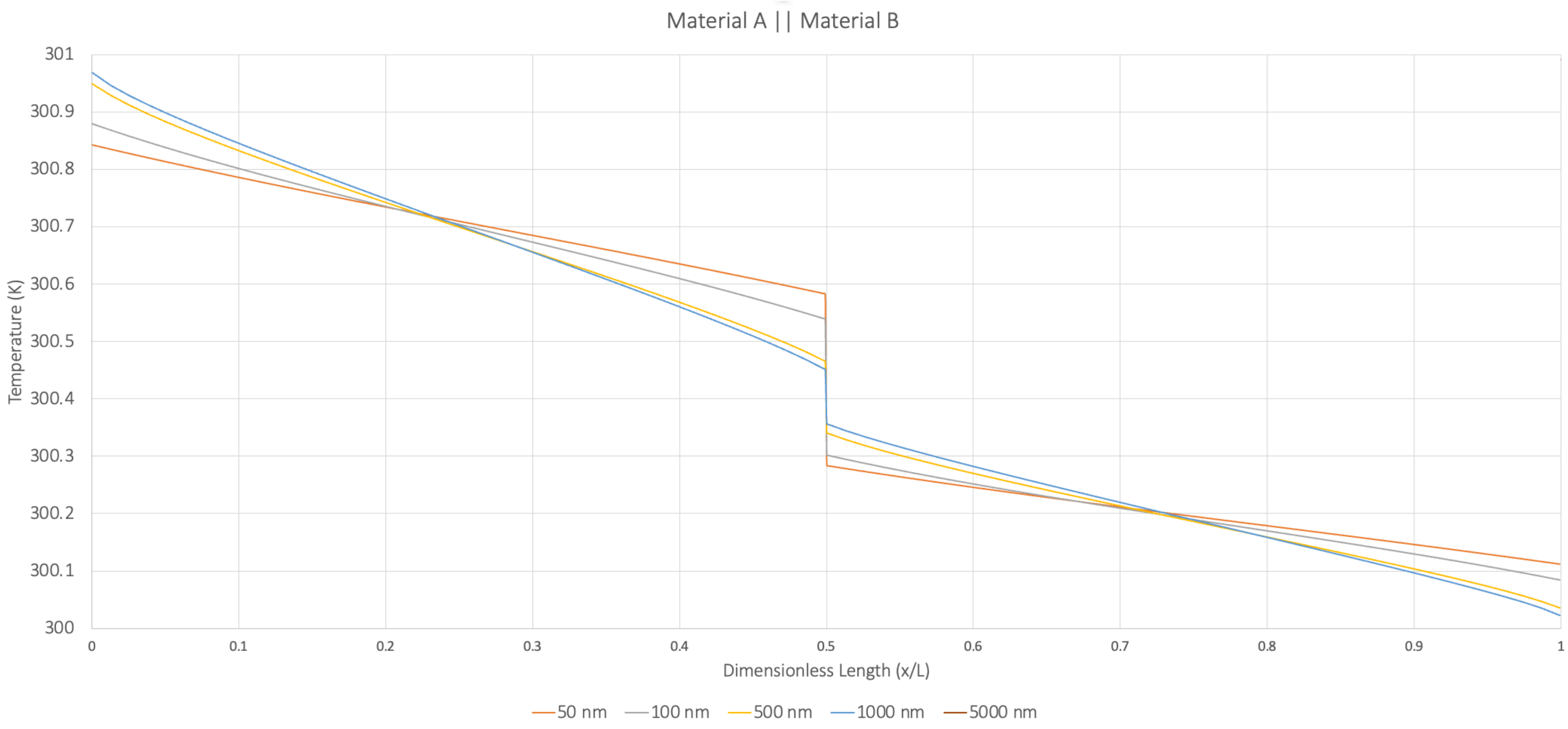


- Temperature determined by contribution of flux from each material, weighted by heat capacity

$$T_{\mathrm{avg.}}\left(\mathbf{r}_{\mathrm{int}}\right) = \frac{\left(\sum_{g^-} C_{g^-,\alpha} T_{g^-,\alpha}\right) + \left(\sum_{g^+} C_{g^+,\delta} T_{g^+,\delta}\right)}{\left(\sum_{g^-} C_{g^-,\alpha}\right) + \left(\sum_{g^+} C_{g^+,\delta}\right)}$$

Thermal interfacial resistance

Spectral transport in test material system

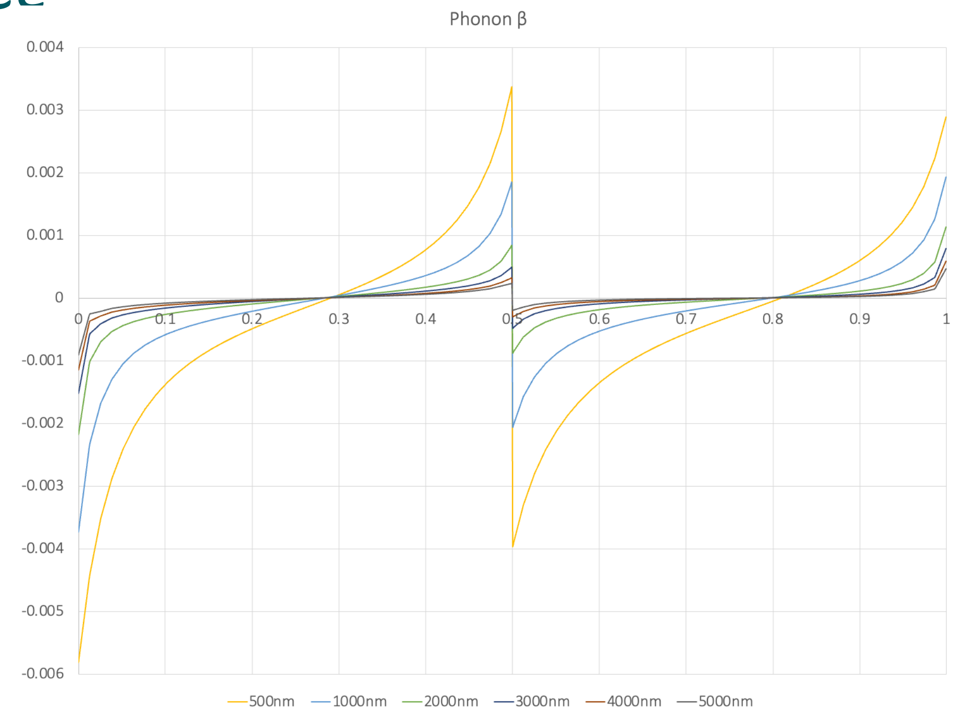


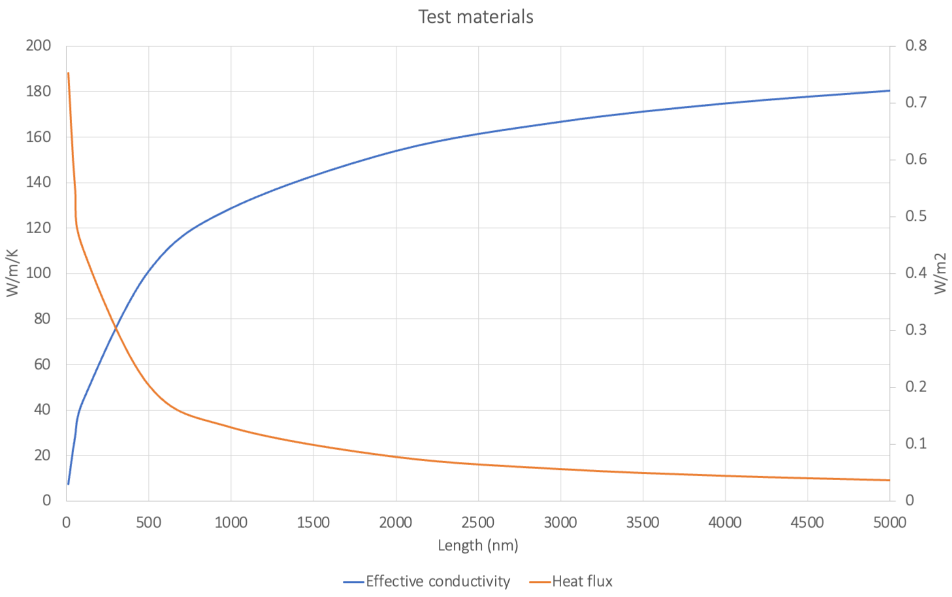
- Temperature slip at interface a function of slab dimension
- Smaller systems out of equilibrium

Thermal interfacial resistance

Spectral transport in test material system

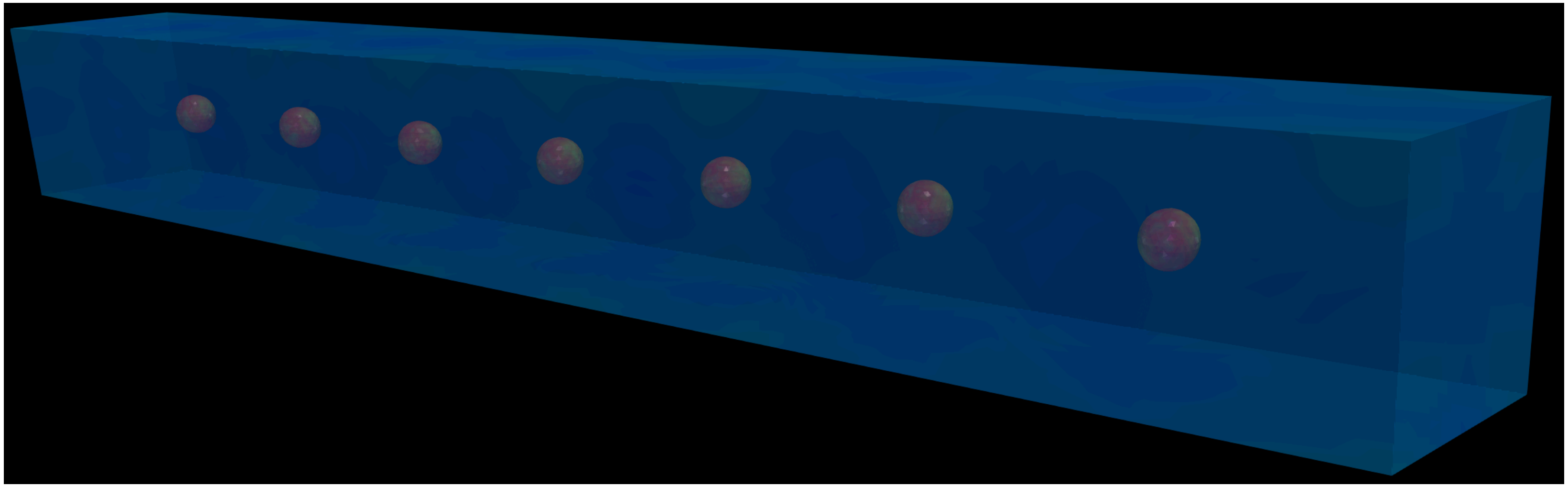
- β is a measure of non-equilibrium behavior
  - Ballistic/diffuse phonon regimes in heterogeneous systems

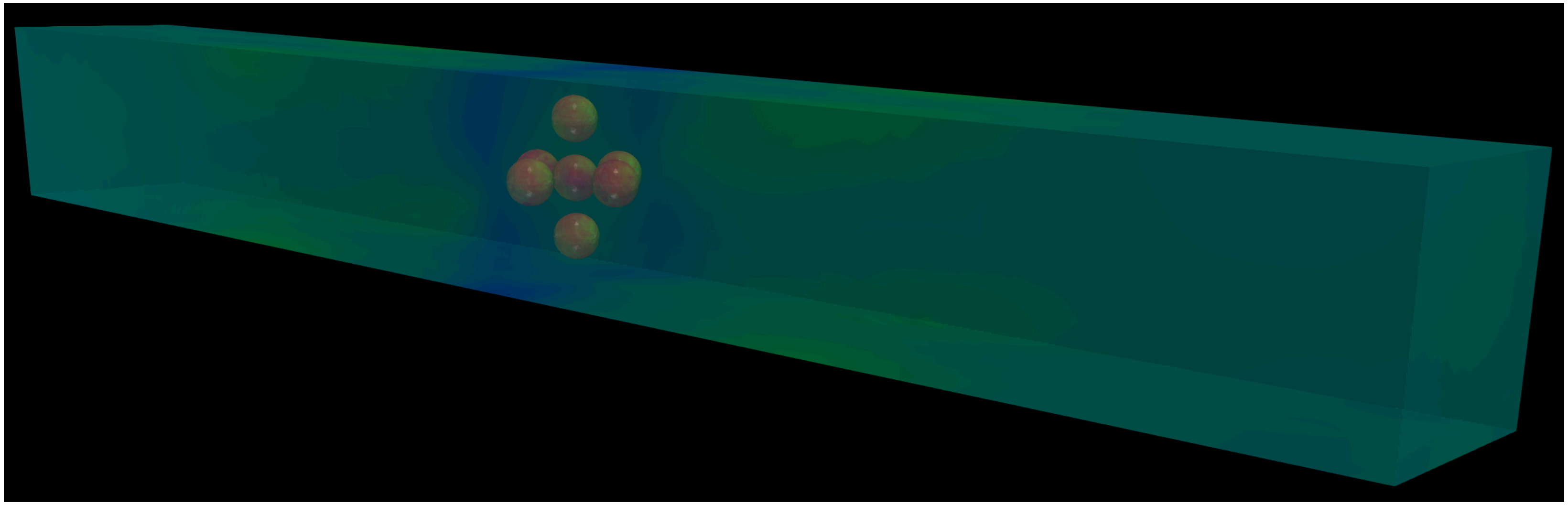




Thermal interfacial resistance

Spectral transport in test material system





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Conclusions

- Requirement to model phonon transport effects at internal interfaces
  - Nuclear reactor simulations generate fission products
- Method general, extendable to non-nuclear applications
- Interface refinement is open research
  - Reality: Finite thickness, structure, voids, p-p interaction, p-e interaction, Sharvin resistance

- 2023 *Boltzmann* release

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