



A First Principles Approach to Spectral Phonon Transport in Heterostructures

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Changing the World's Energy Future

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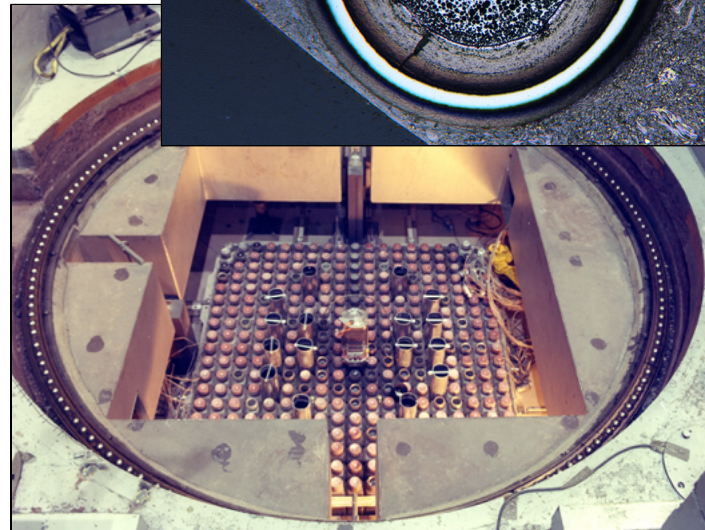
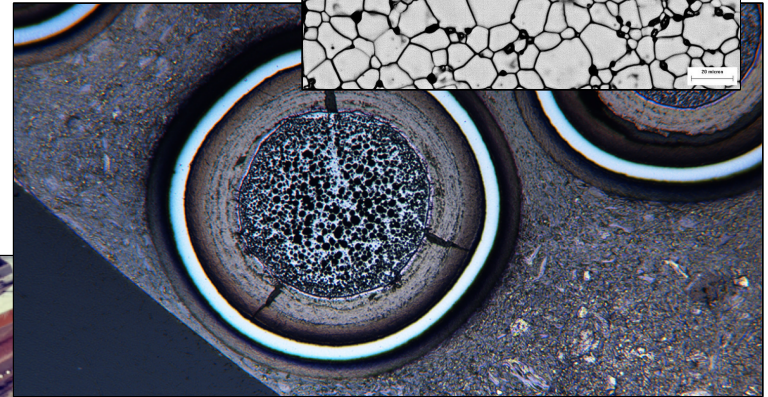
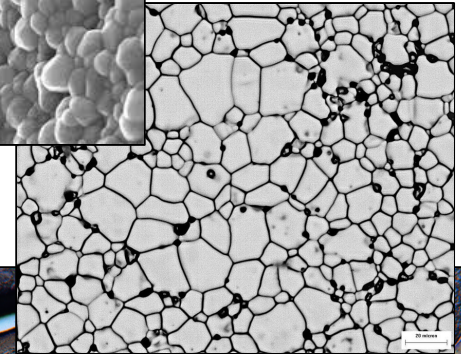
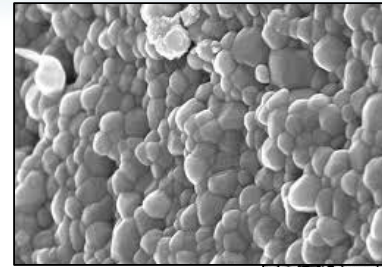
Outline

- 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

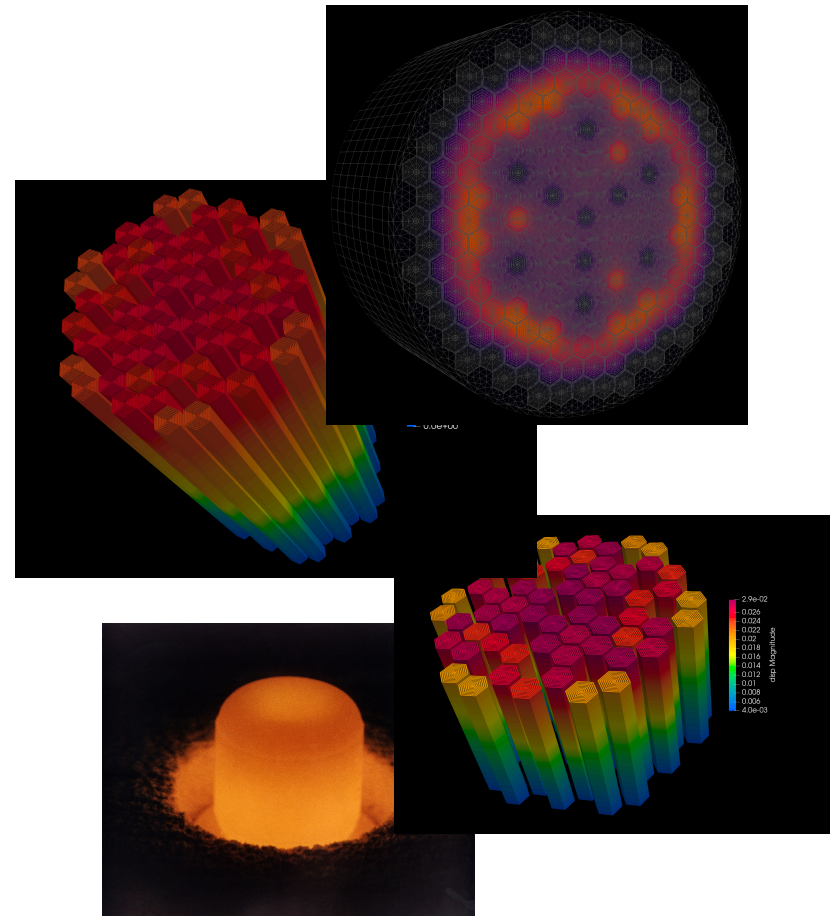


Motivation

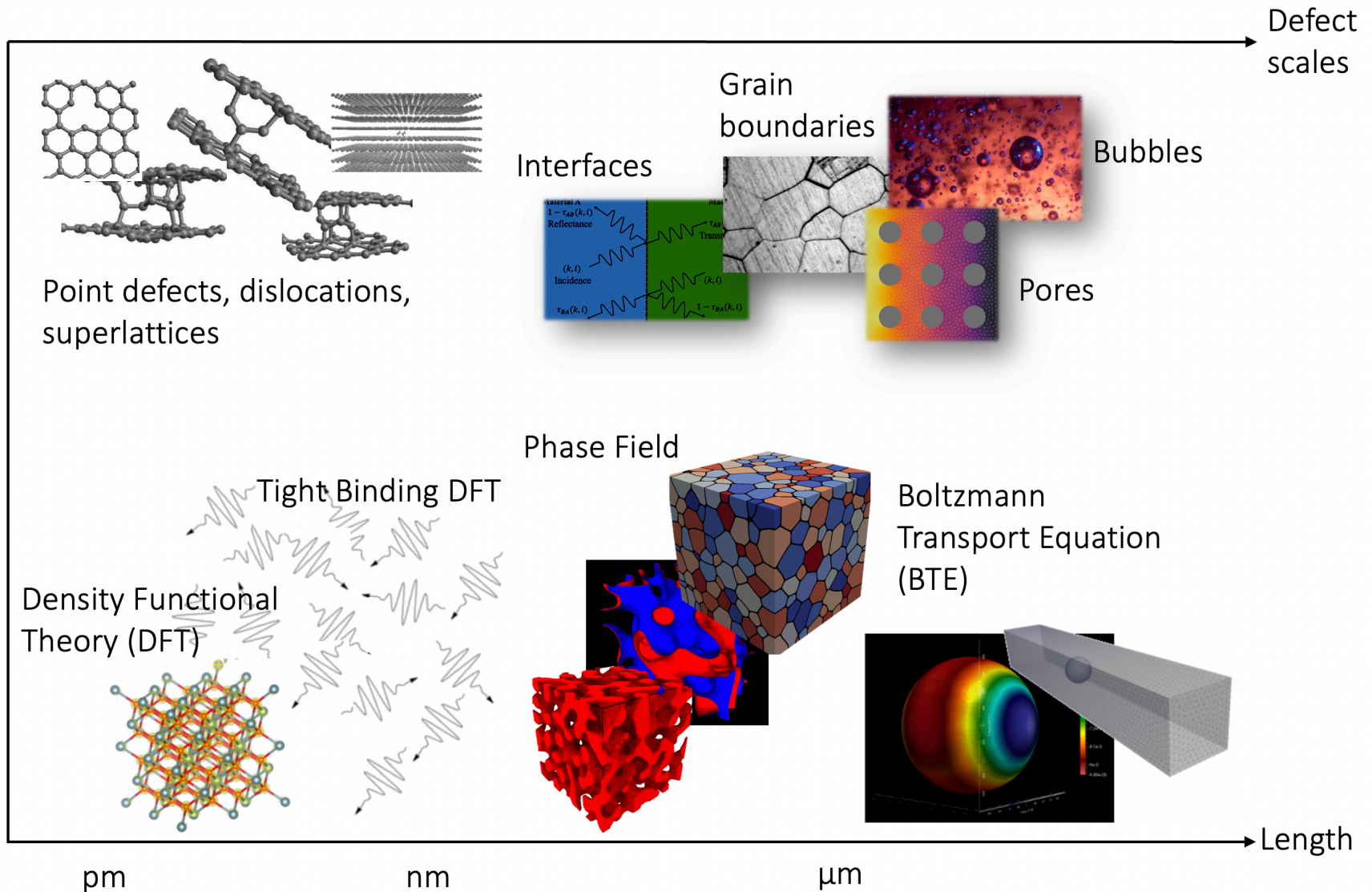
Nuclear reactor fuel performance

- 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

MOOSE



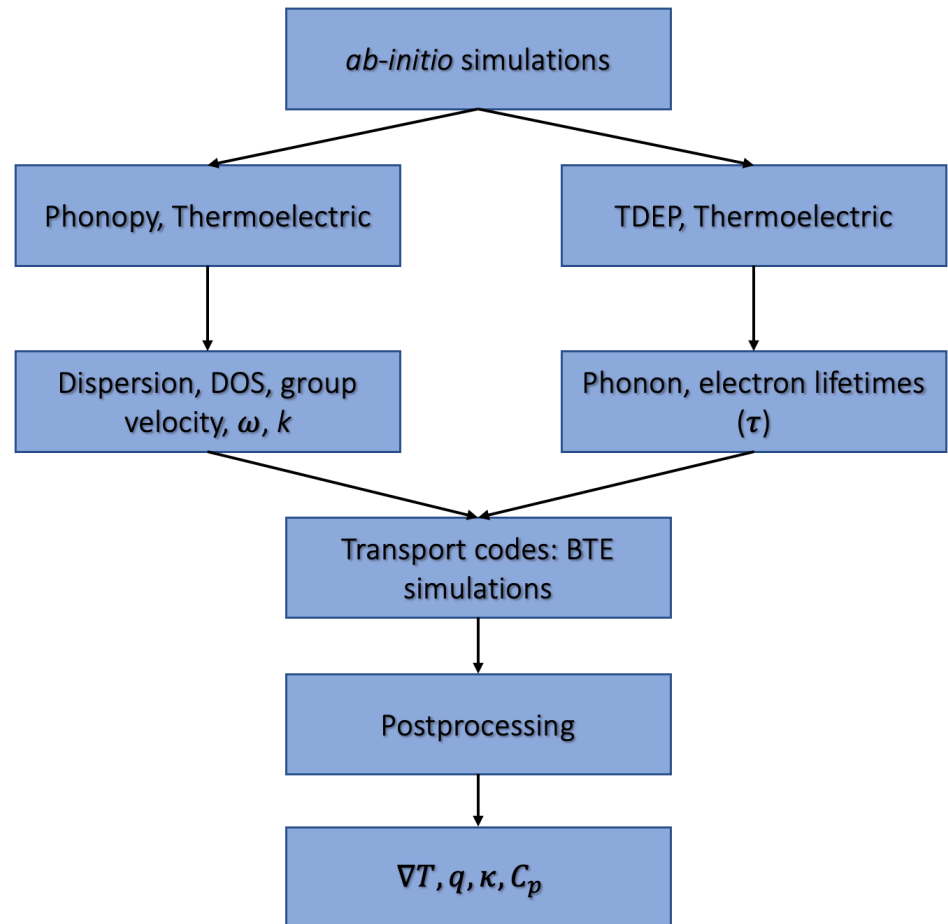
Scale and defect regimes in heat transport



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

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

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

- Temperature phonon $\phi_g^T = \sum_{m=1}^M \psi_{m,g} w_m$ d with a func $\phi^0 = \phi^0 \left(T(\mathbf{r}), \hat{\Omega}, \xi, p \right) = \frac{\hbar \omega \mathbf{v} \mathbb{D} d\eta}{\exp \left[\frac{\hbar \omega}{k_B T(\mathbf{r})} \right] - 1}$

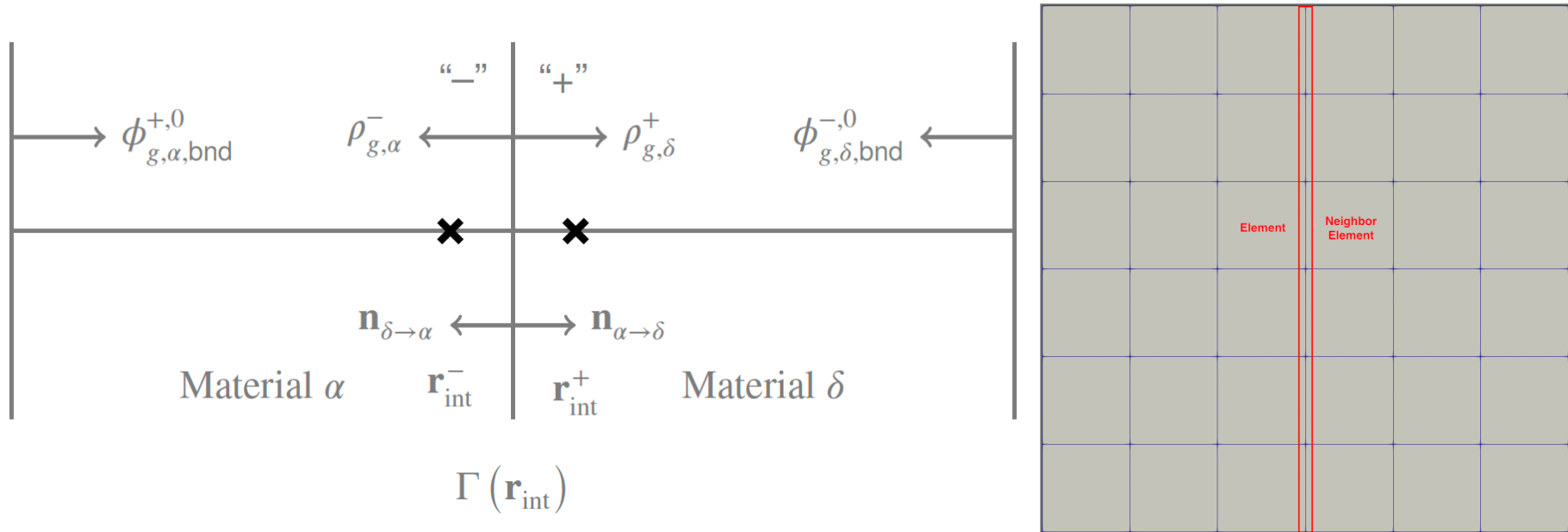
$$T_g(\mathbf{r}) = \frac{1}{k_B} \frac{\hbar \omega_g}{\ln \left[\frac{\hbar \omega_g v_g \mathbb{D}_g}{\phi_g^T(\mathbf{r})} + 1 \right]}$$

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

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

Thermal interfacial resistance

Interface physics

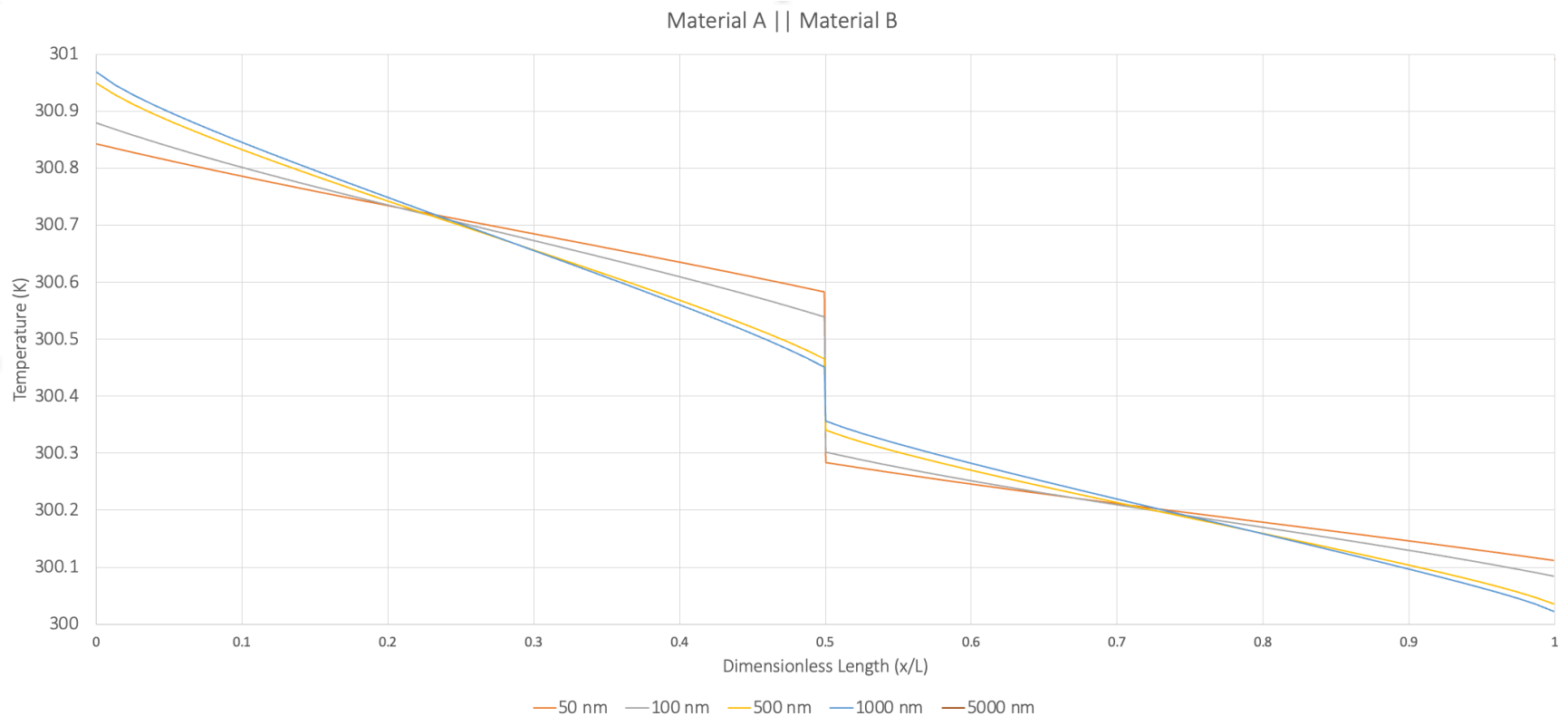


- Temperature determined by contribution of flux from each material, weighted by heat capacity

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

Thermal interfacial resistance

Spectral transport in test material system

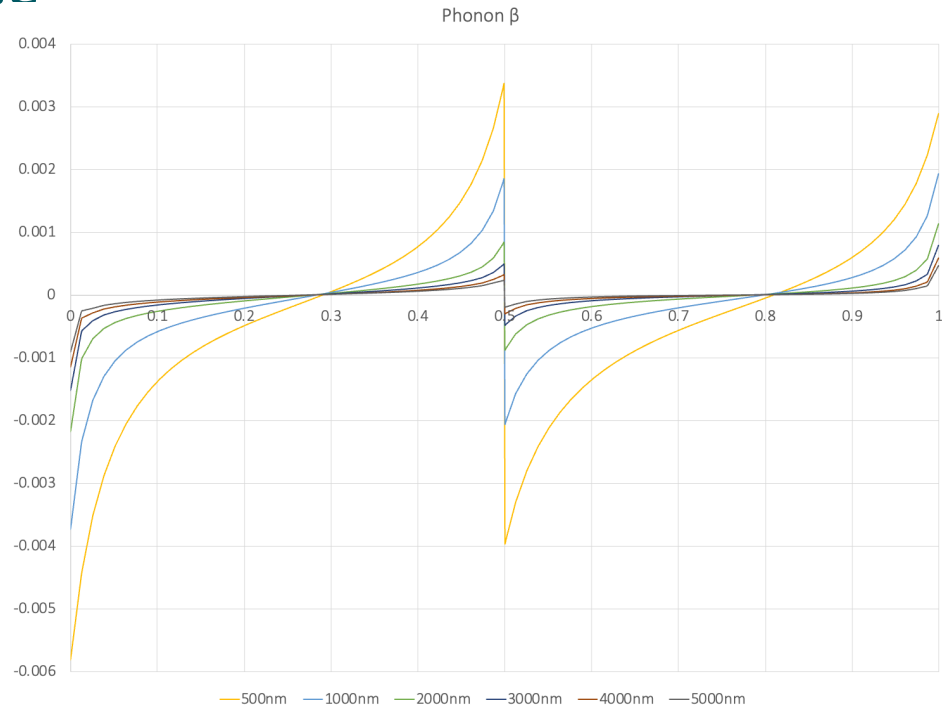
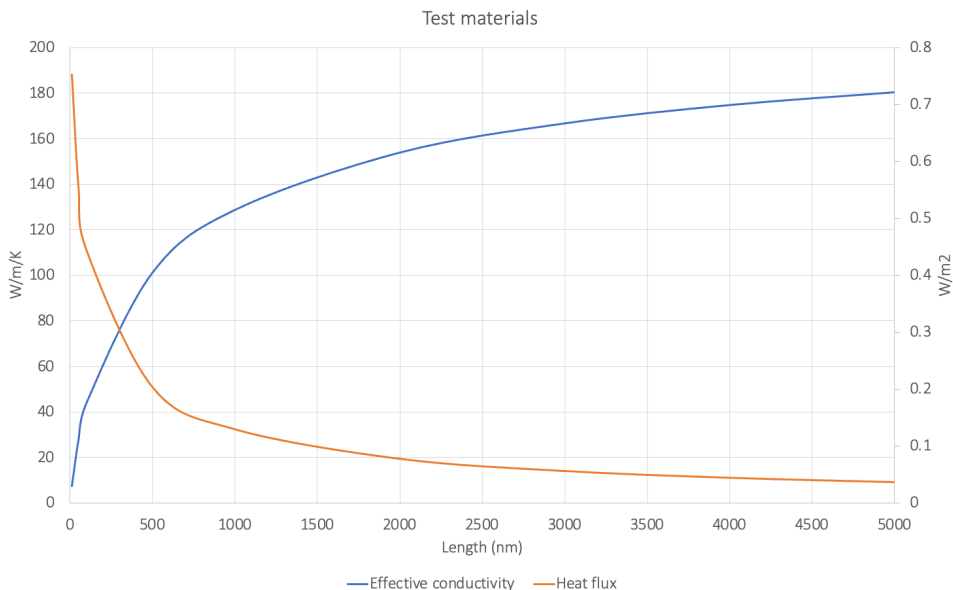


- Temperature slip at interface a function of slab dimension
- Smaller systems out of equilibrium

Thermal interfacial resistance

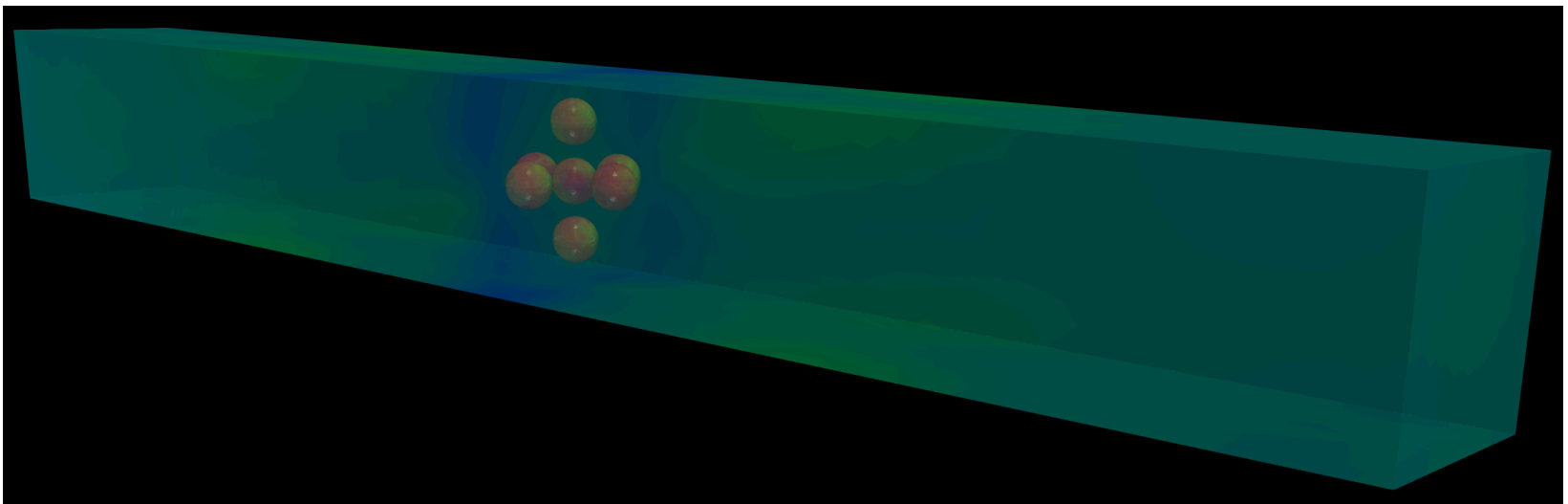
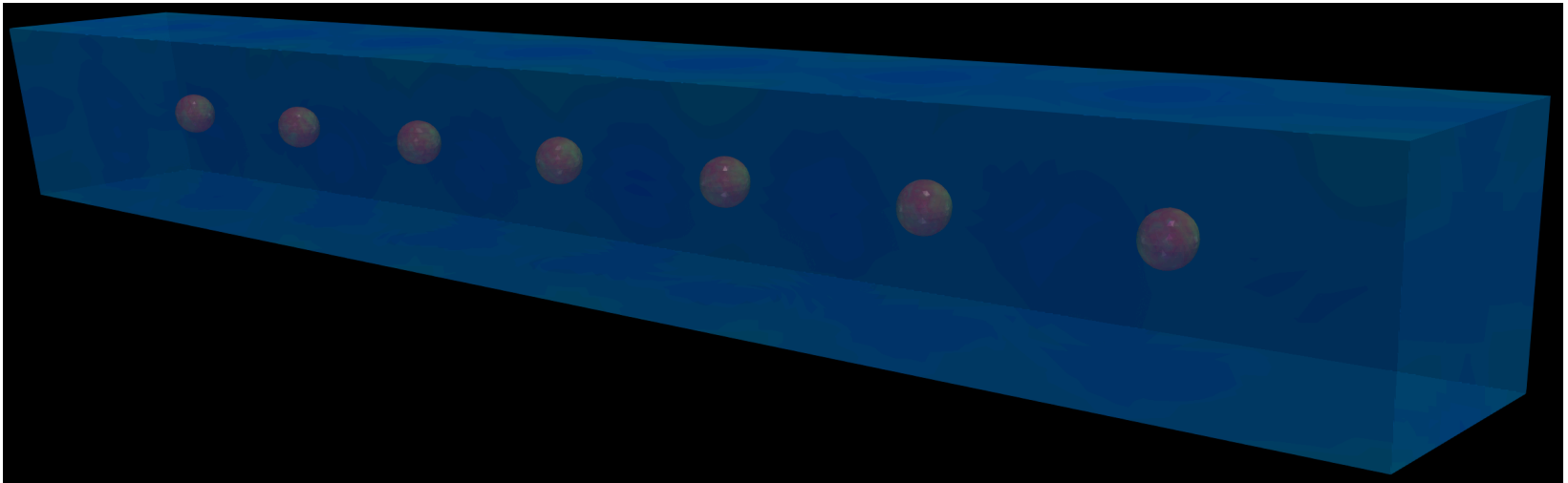
Spectral transport in test material system

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



Thermal interfacial resistance

Spectral transport in test material system



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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