INL/MIS-22-70358-Revision-0

Morphological-informed Thermal Property Prediction in the Engineering Domain

November 2022

Changing the World's Energy Future

Jackson R Harter

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Morphological-informed Thermal Property Prediction in the Engineering Domain

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INL/MIS-22-70358

Introduction

- Who am I?
- Not a good student growing up
- I went to culinary school after high school
  - Worked in restaurants for many years, taught culinary school
- Enrolled at Oregon State University in 2009 at 25, received doctorate in 2019
- Intern at INL summer 2015, 2016, 2018
  - Hired as staff January 2020

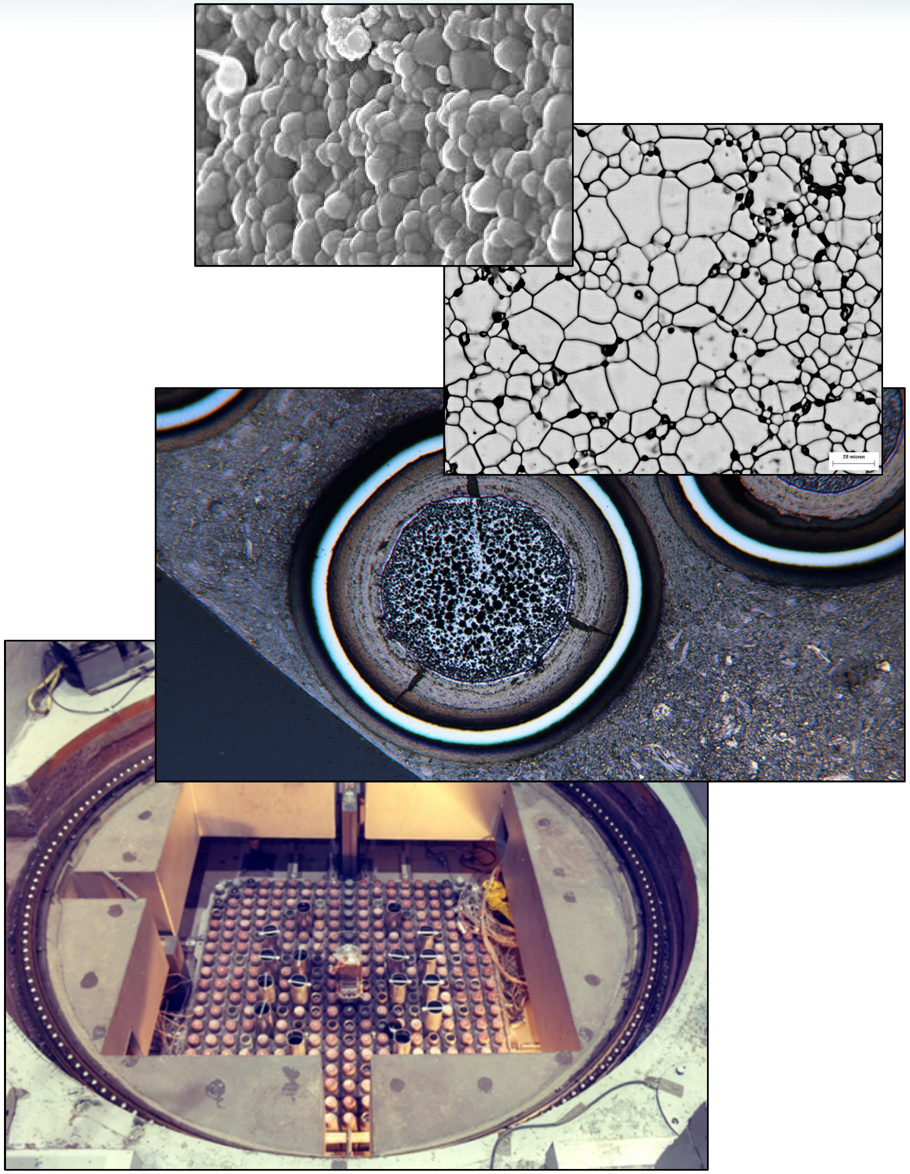
Outline

- Motivation and applications of microscale heat transport
- Phonons and thermal electrons
  - Length scale dependence of thermal properties
  - Physics & methods of microscale heat transport
  - Thermal interface resistance
  - Code development
- Thermal properties from atomic scale to engineering scale
  - Importance
  - Precision multiphysics and multiscale methods

Motivation

Thermal properties

- Insights on thermal properties are critical to understanding thermal performance



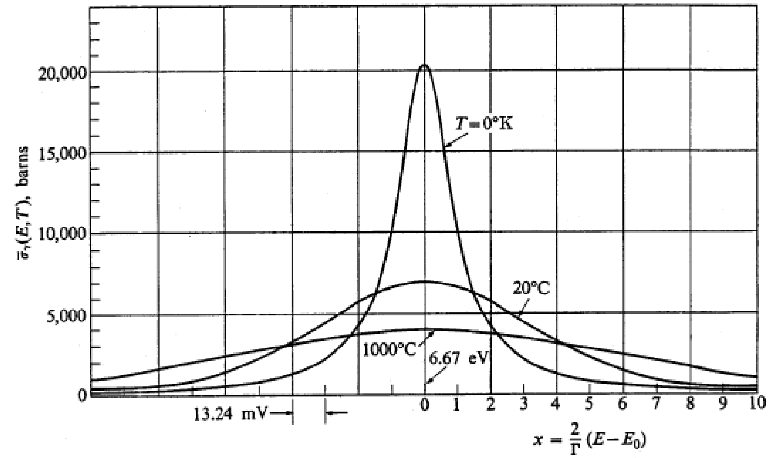
- But these *macroscopic* quantities used in engineering applications are affected by changes at the *microstructural* and *atomic* level

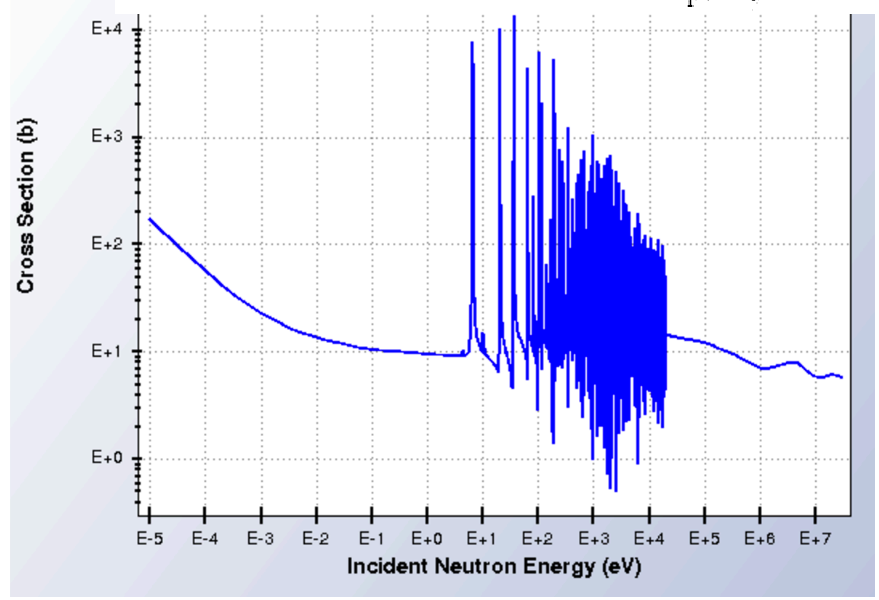
Motivation

Applications in nuclear science

- The neutron interaction cross section is highly influences by changes in temperature
  - Change in target size

contraction

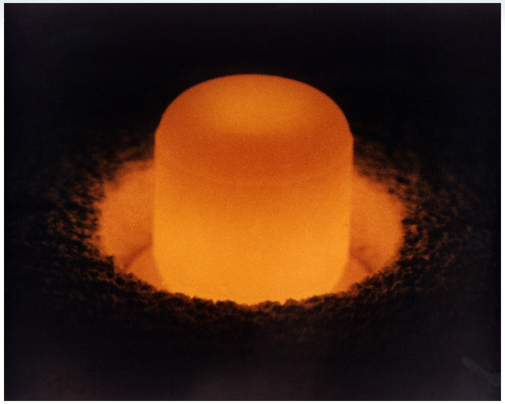


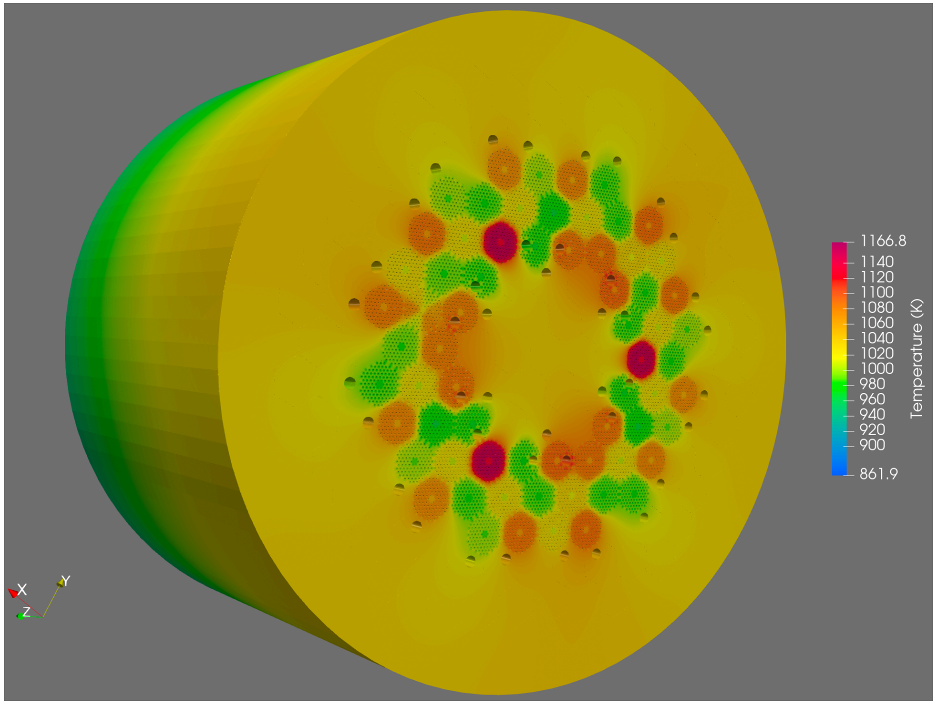


Motivation

Nuclear reactor fuel performance

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

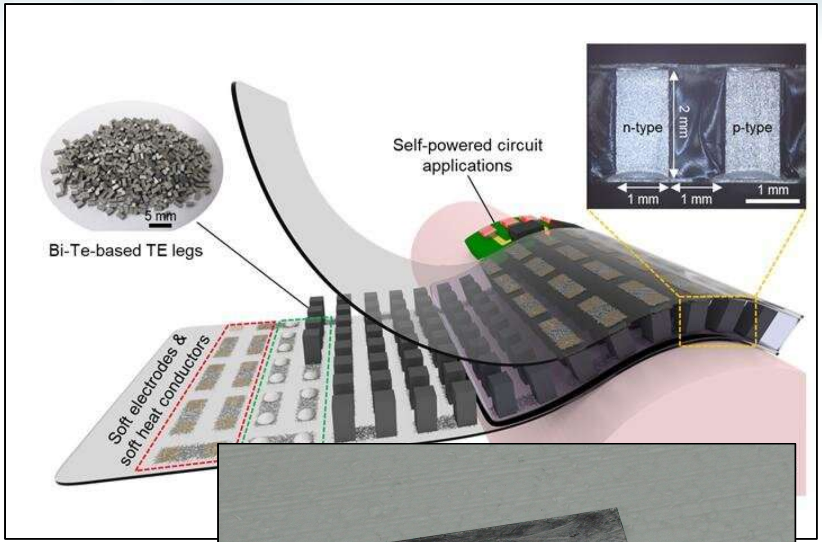


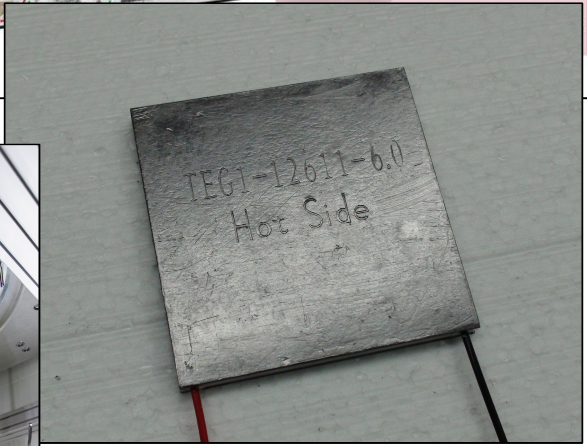


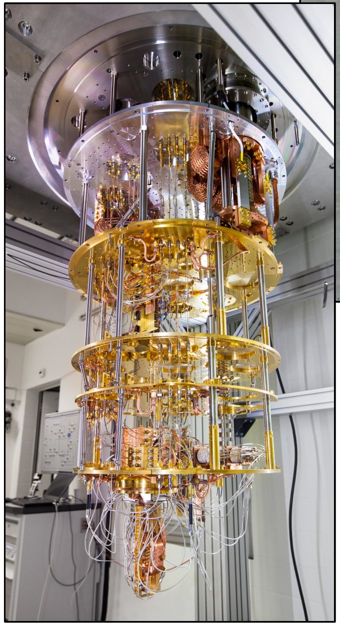
Motivation

Thermoelectric devices and more

- Thermoelectric devices
  - Seebeck effect
  - Recycling waste heat to produce electricity
  - Remote nanosensors
- Thermal management in traditional and quantum computing
  - Devices need to be kept at certain temperatures in order to perform



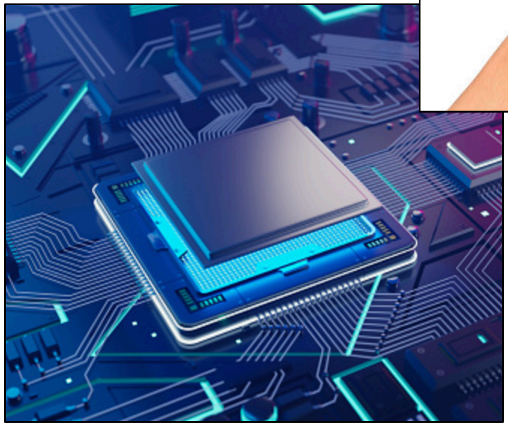




Motivation

Assisting new research and development

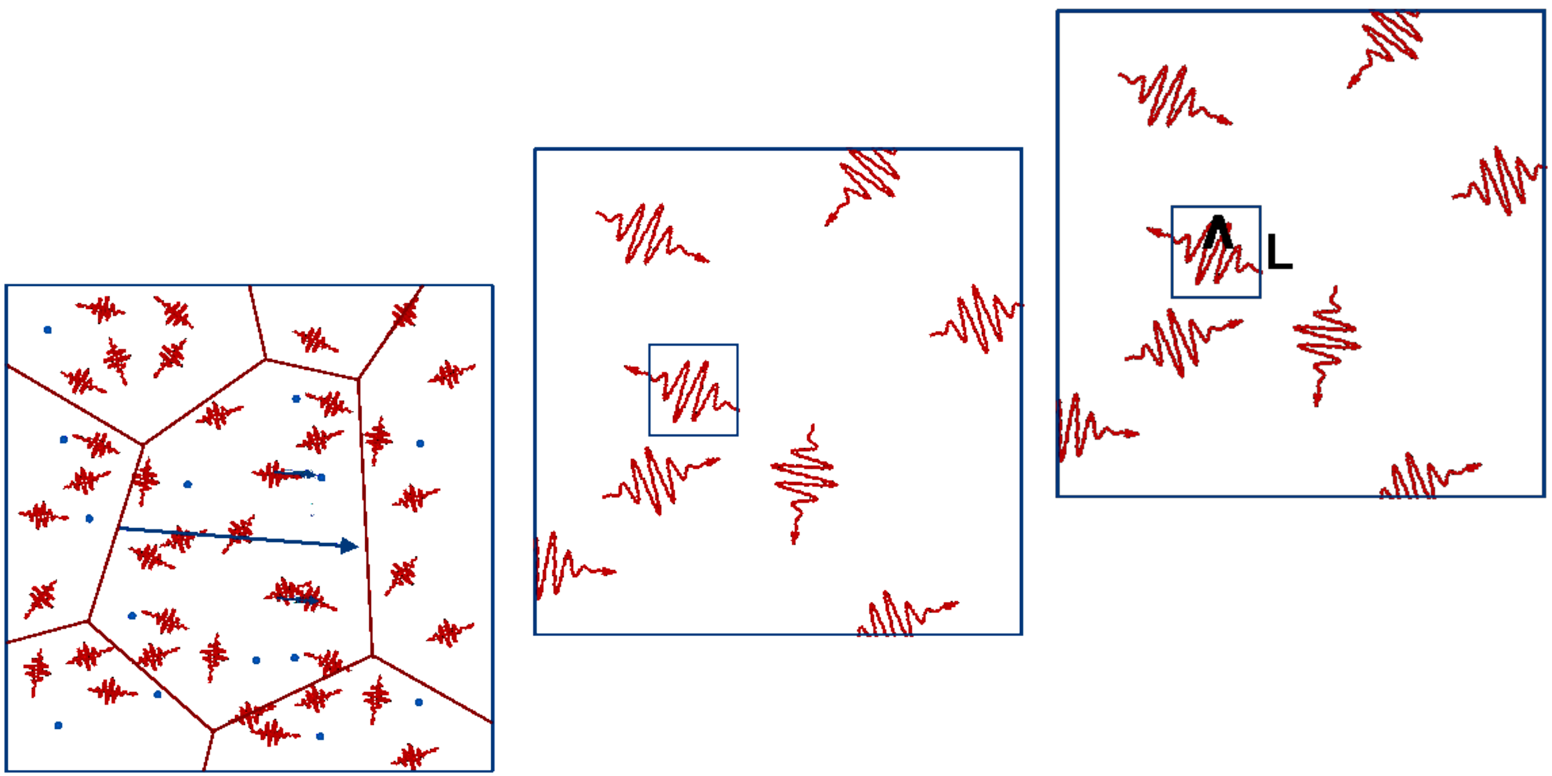
- Reduce the need for expensive experimentation
  - Work by Majumdar in 1990s on microscale thermal transport
- Increasing speed of development of new materials and devices
  - Narrow window of experimentation
  - Reduce costs, allow for less expensive fabrication
- How is this done?



Mechanistic prediction of thermal properties

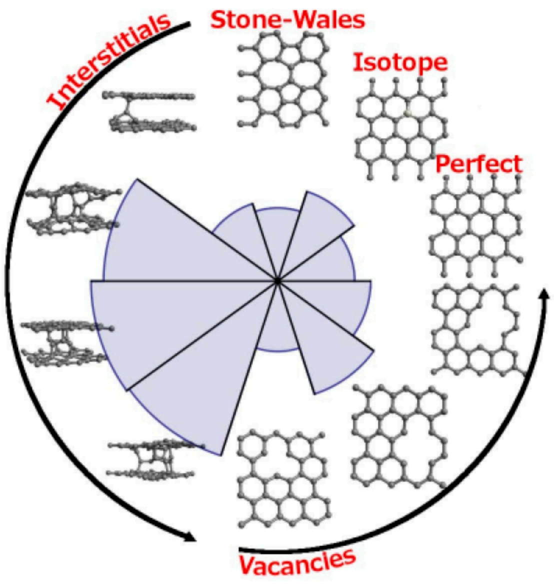
Conduction at the atomic scale

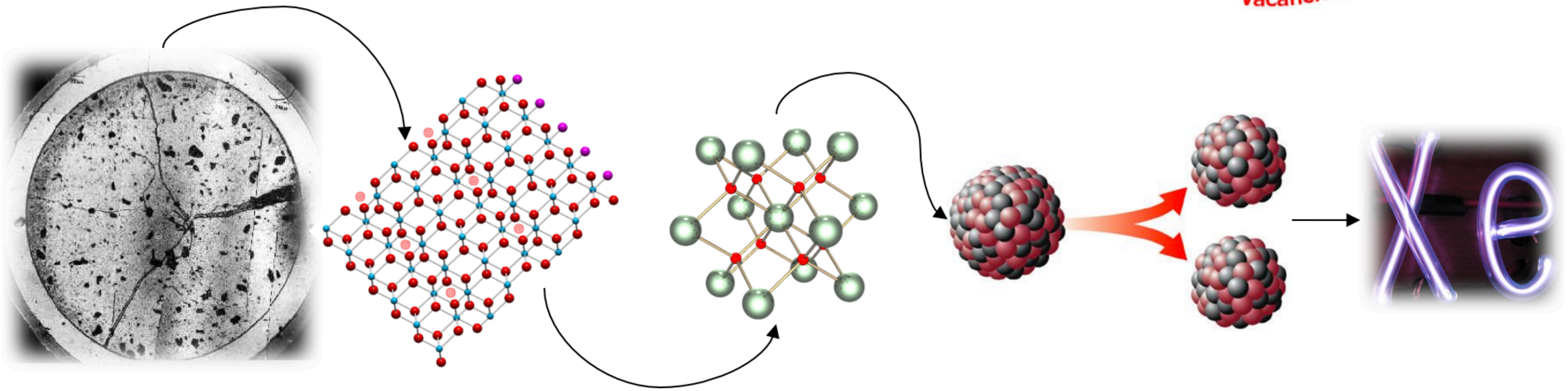
- Transporters of thermal energy
  - Electrons (metallics)
  - Phonons (dielectrics and insulators)



Defect influence on thermal transport

- What are defects?
  - Structural anomalies in the atomic lattice
- Defect presence causes increased phonon and electron scattering, lowering heat flux and thermal conductivity
- This is a complex, *multiphysics* challenge





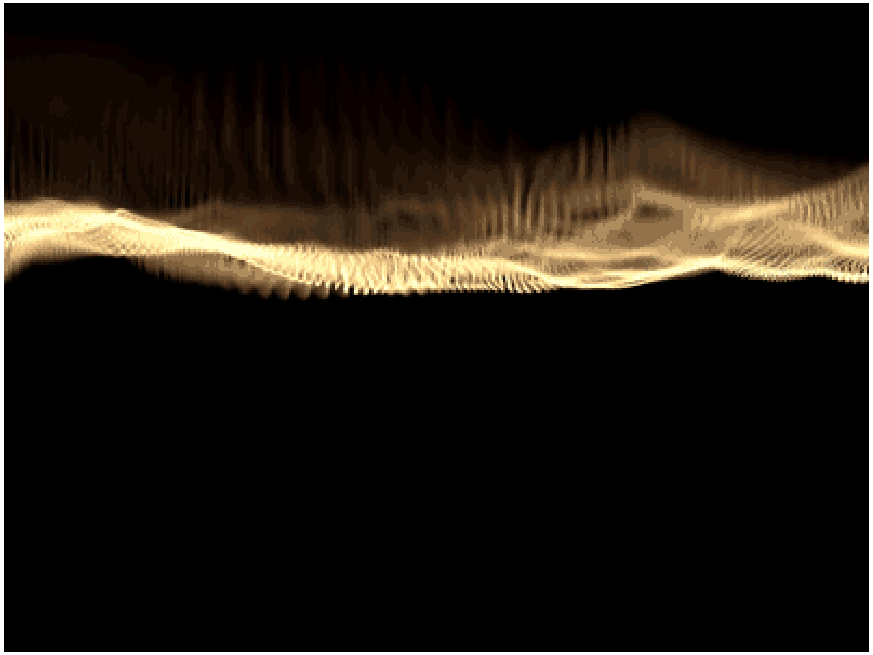
Why should you care?

Our (lack of) understanding of materials behavior is a limiting factor in all engineering disciplines

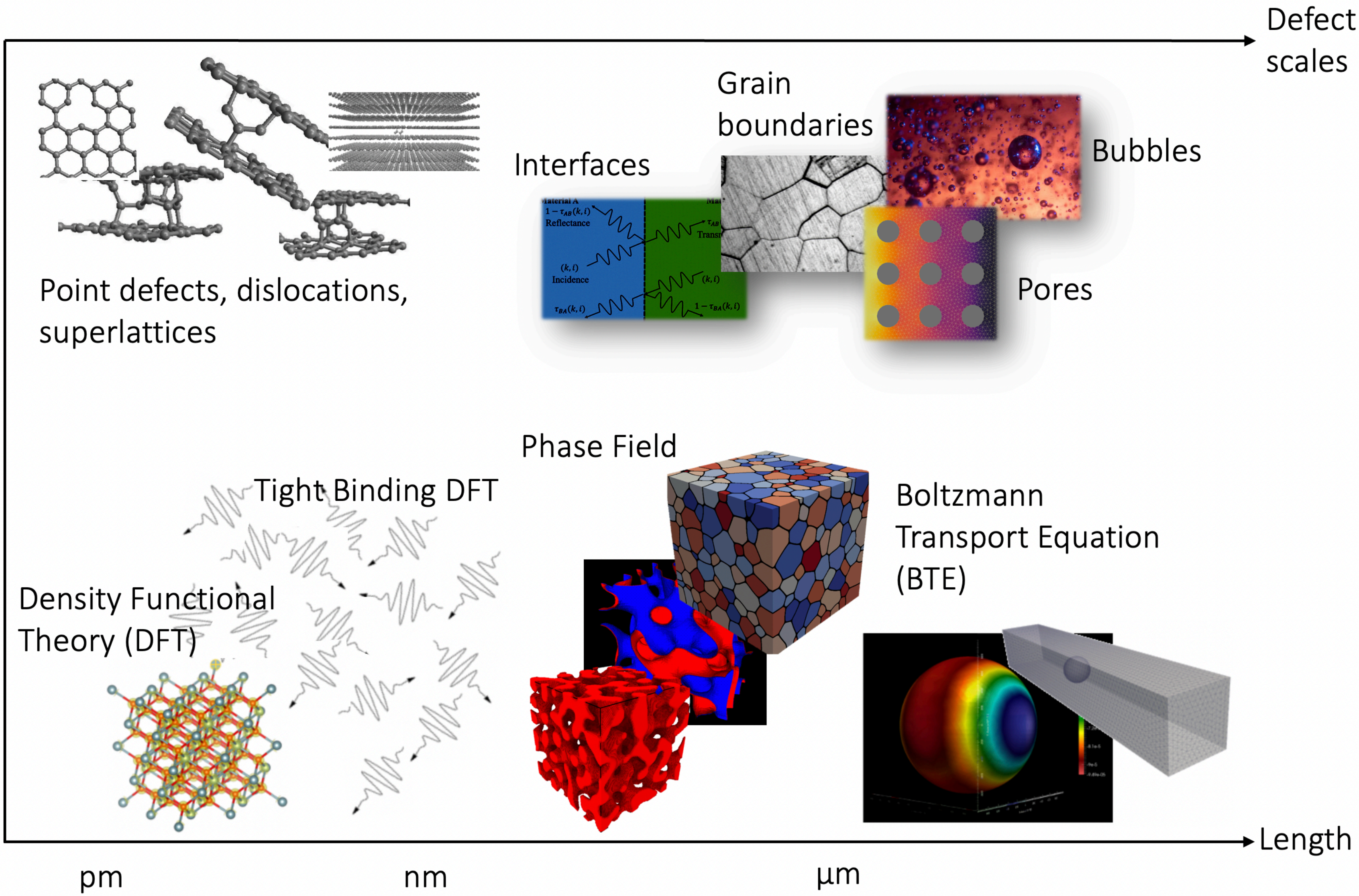
Overview

What are phonons and electrons?

- For materials in the solid state a vibrational spectrum ω exists
  - Phonons are generated via atomic displacements
  - Phonons are quantized waves, simulated as quasi-particles
  - Follow Bose-Einstein statistics
- Electrons are also simulated as quasi-particles
  - Not generated from displacements, but moved through thermal and electrical influence
  - Follow Fermi-Dirac statistics

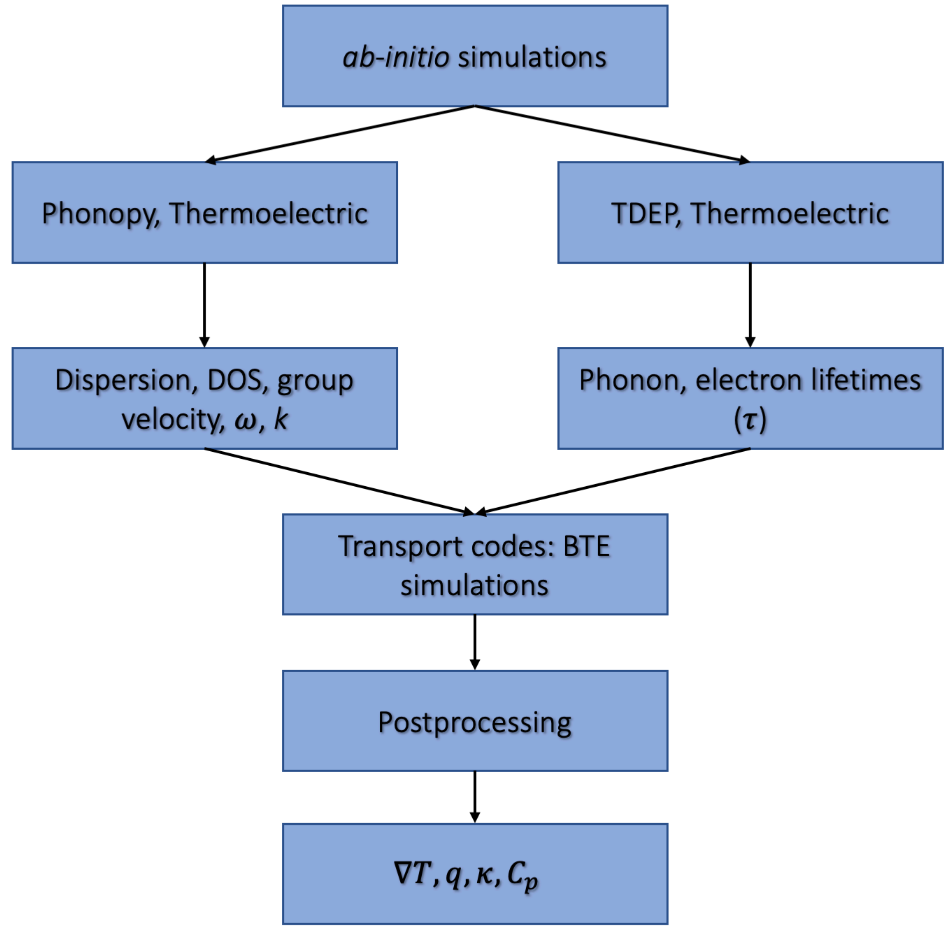


Scale and defect regimes in heat transport



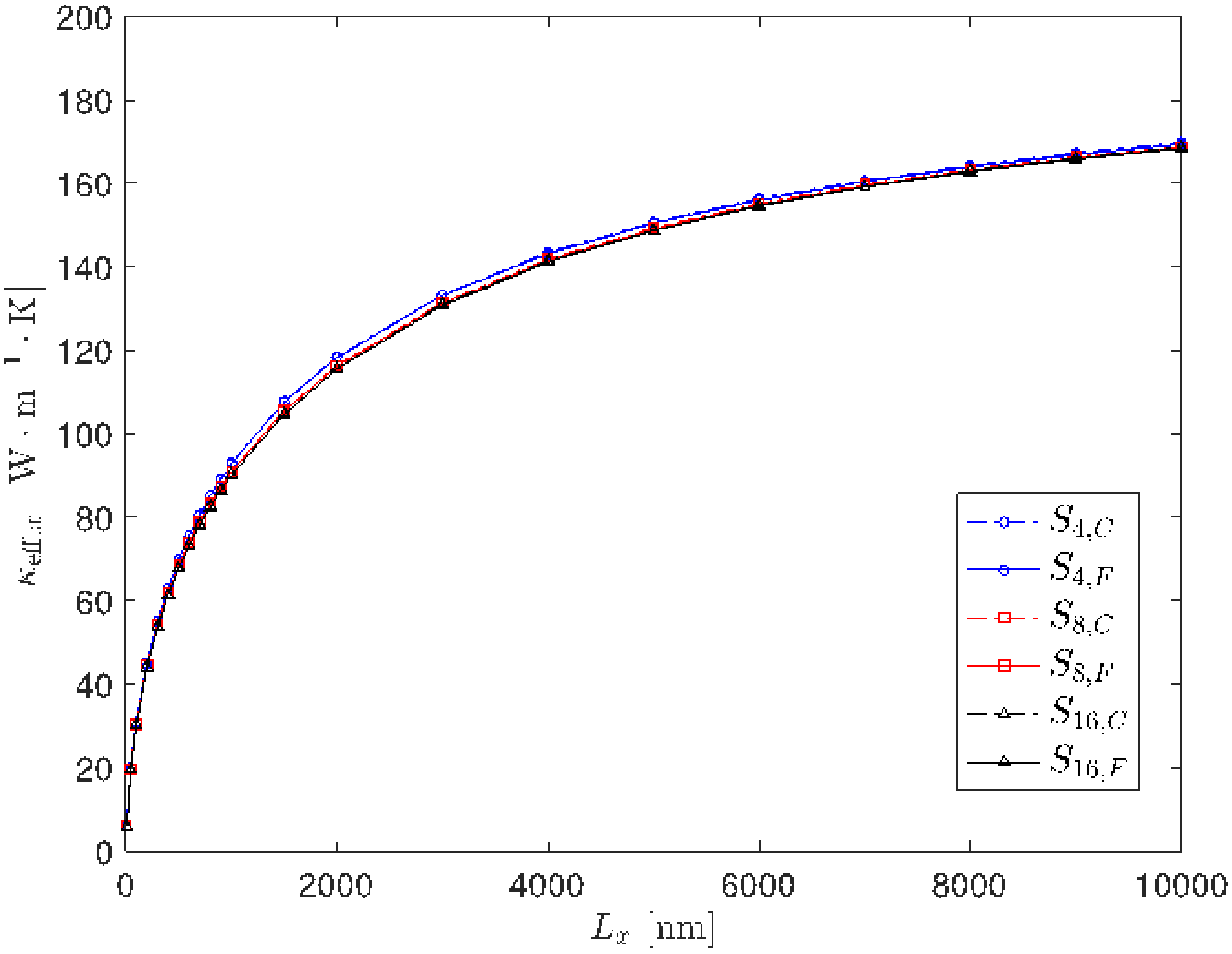
Heat transport workflow

- *ab-initio* simulations
  - Phonon/electron dispersion
  - Density of states
  - Relaxation times
  - Everything at 0 Kelvin!
- Material properties into transport codes
- BTE simulations
- Results ⍰ heat flux, thermal conductivity, temperature distributions, heat capacity
  - Stop here or pass values to other code in multiphysics simulation
- Preprocessing, postprocessing



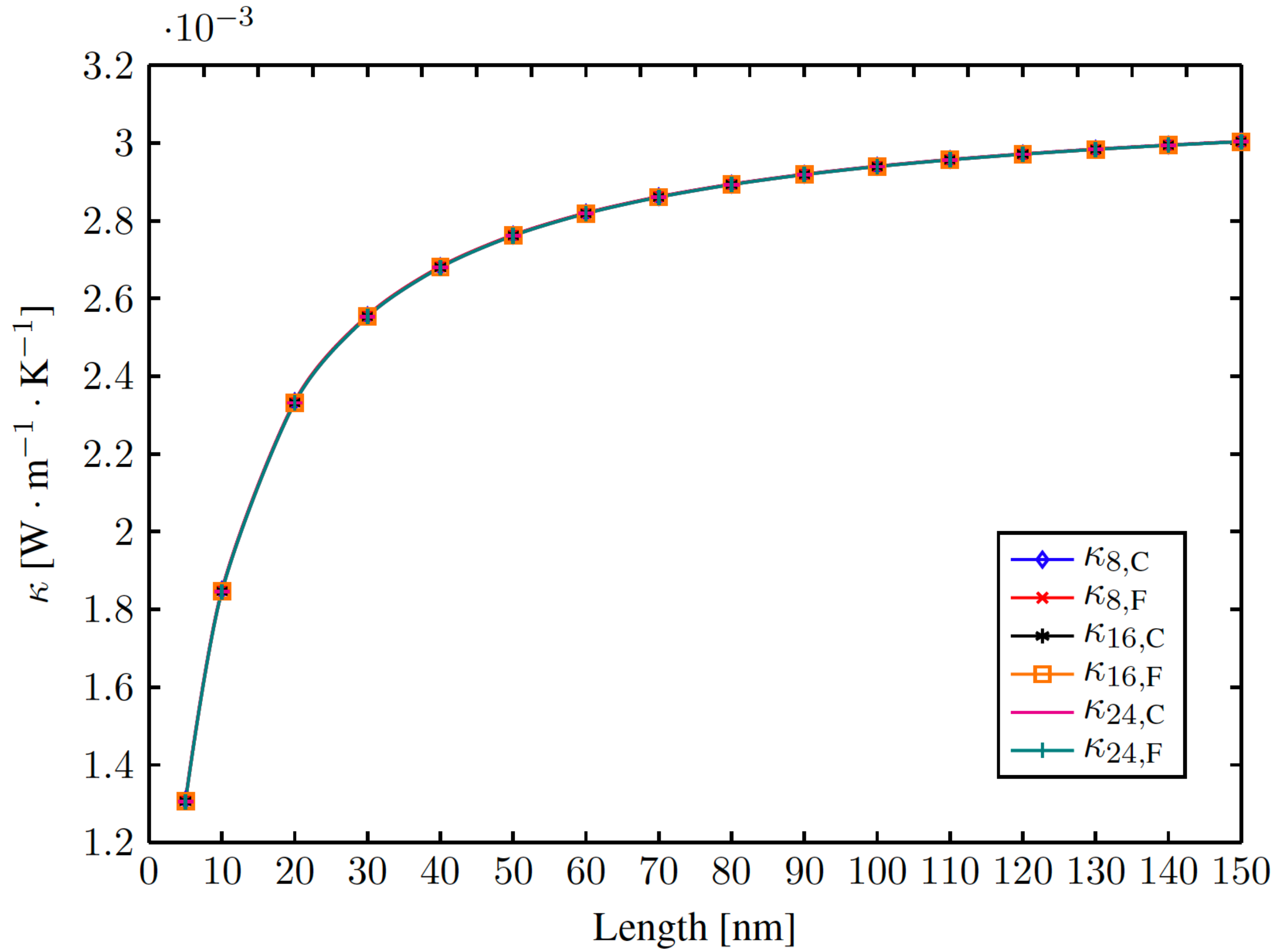
Length scale dependence of

Phonons



Length scale dependence of

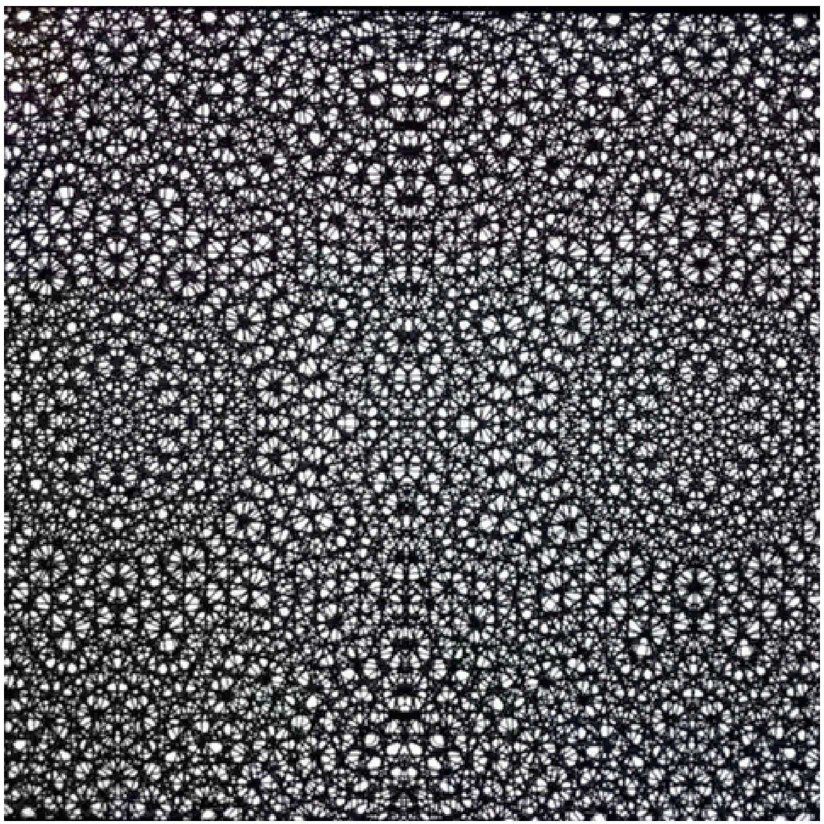
Electrons

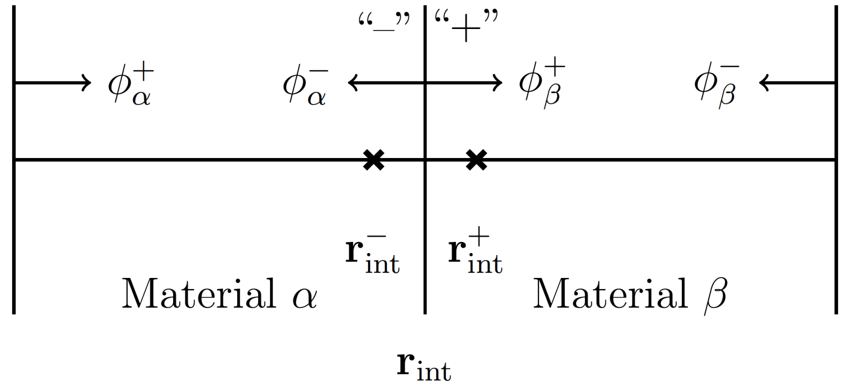


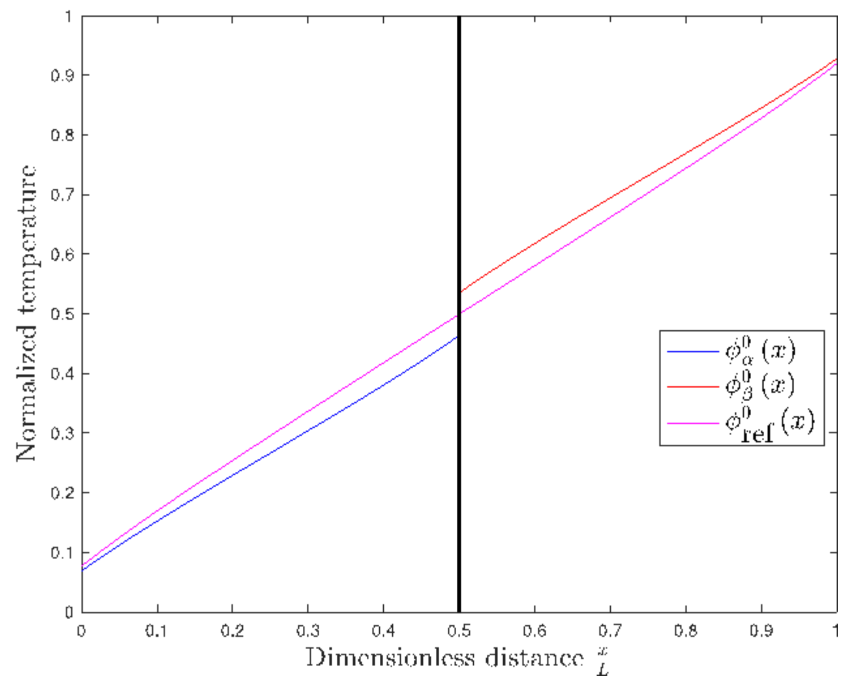
Thermal interfacial resistance

Interface physics

- Phonons experience resistive effects at physical interfaces in materials



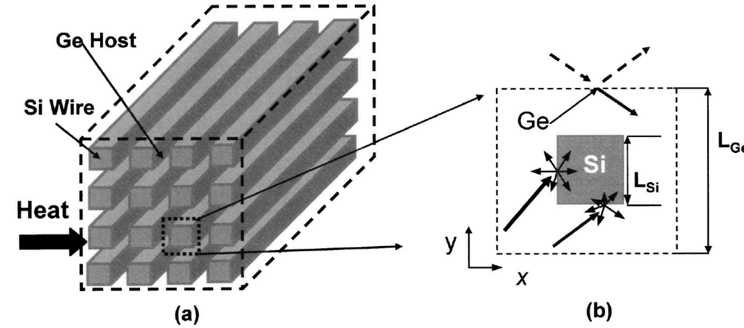


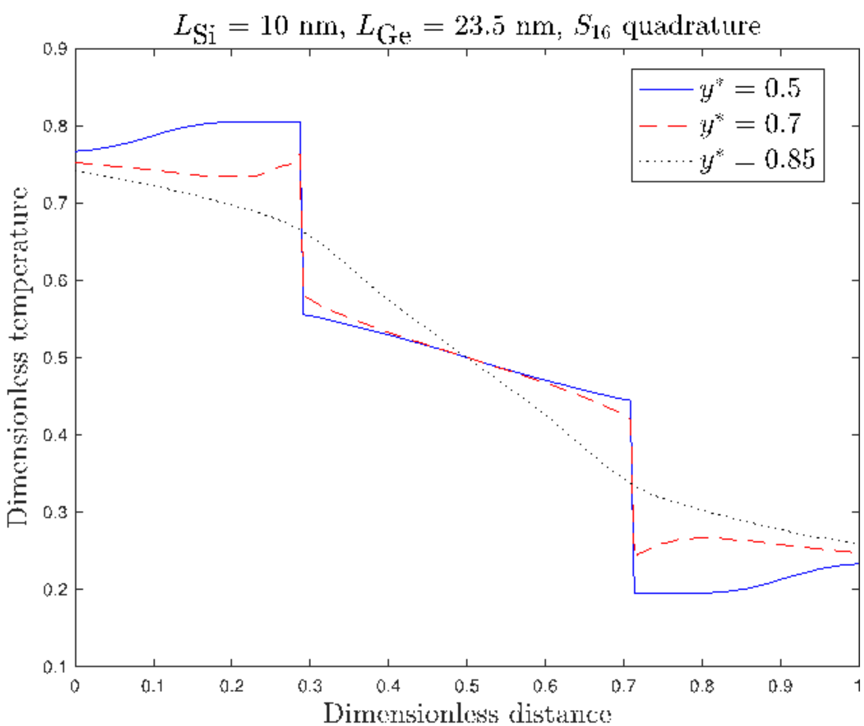


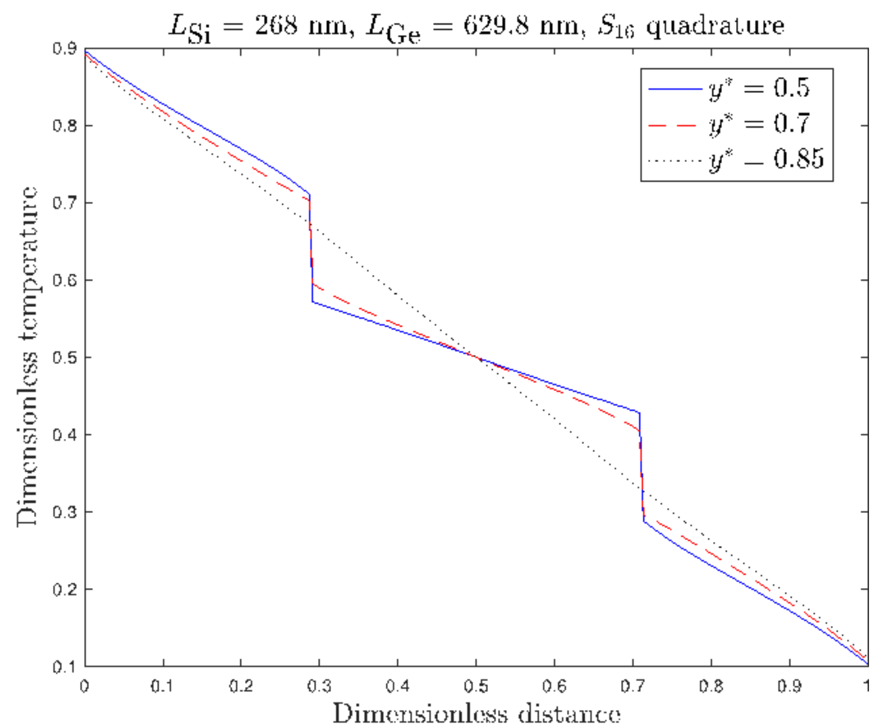
Thermal interfacial resistance

Code verification in Si-Ge system

- Yang & Chen 2D simulations of Si nanowires in Ge host
  - Phys. Rev. B **69** (2014)
- Reproduces , ,



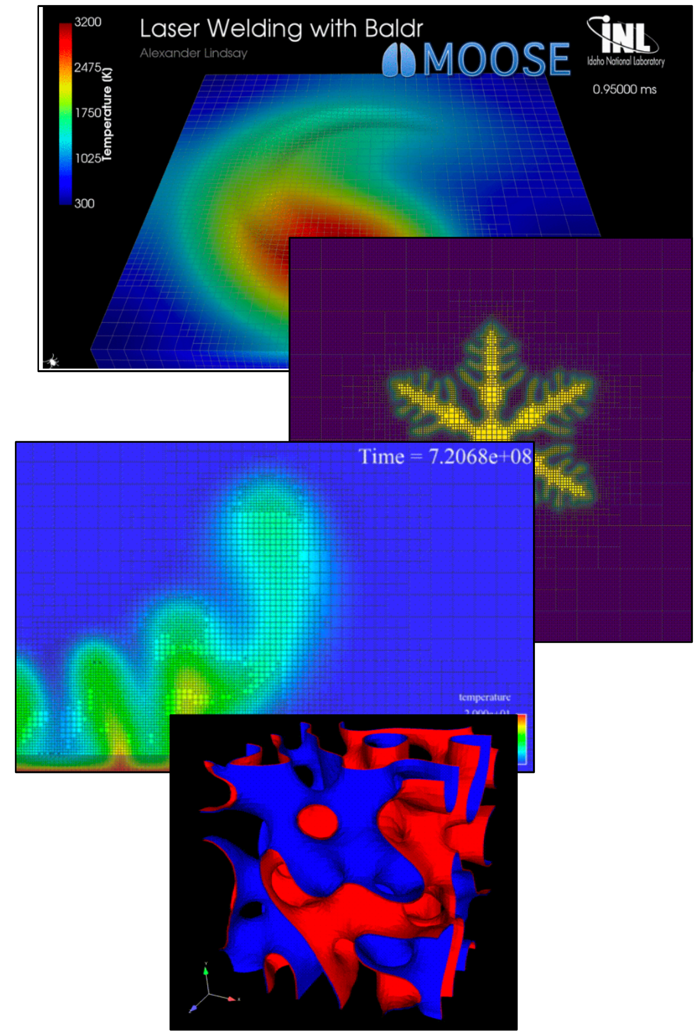




Code development

Creation of Boltzmann module

- *Boltzmann* combines phonon and electron transport with machinery designed and incorporated in *Griffin*, a radiation transport code
- These codes are built on the MOOSE framework, conceived and developed at Idaho National Laboratory



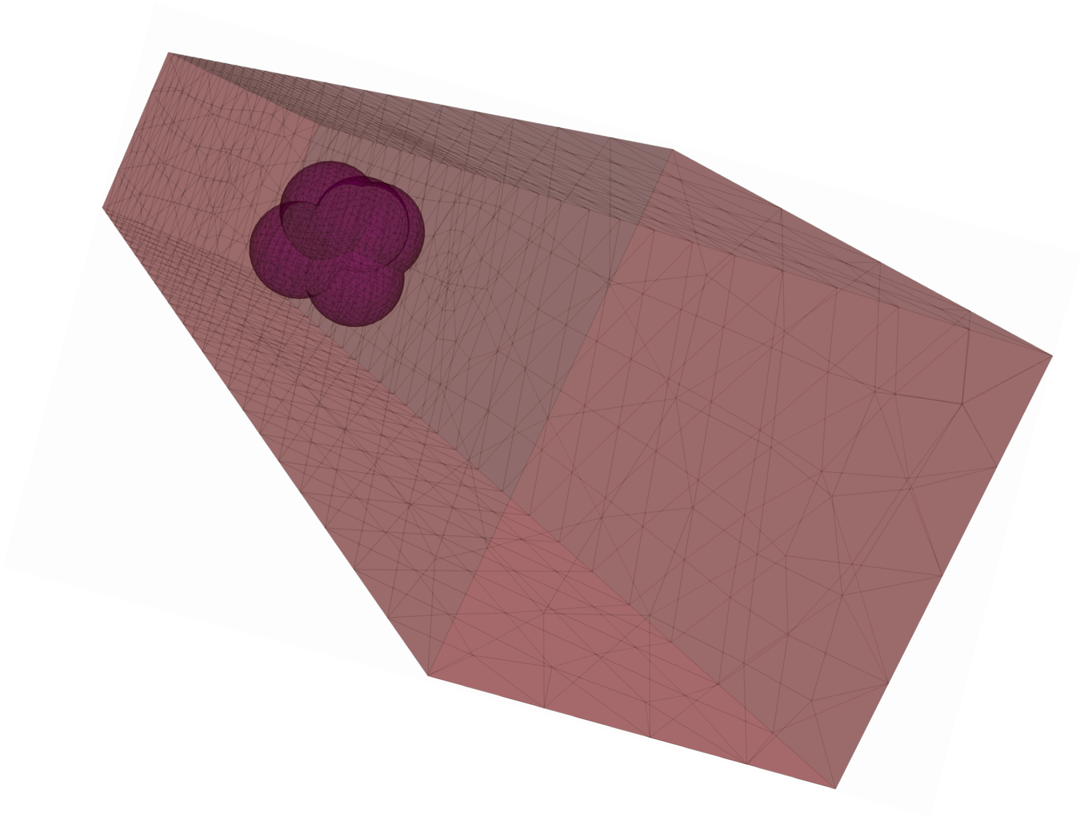
Funding sources

- This work has been supported through
- Seed LDRD 20A1049-012FP: Multiscale thermal properties prediction in MOOSE via a general Boltzmann solver (FY20->FY21). Role: PI
- LDRD 21A1050-052FP: Accelerating pathways to actinide materials discovery through combinatorial deposition (FY21->FY23). Role: Co-I

Examples of phonon transport

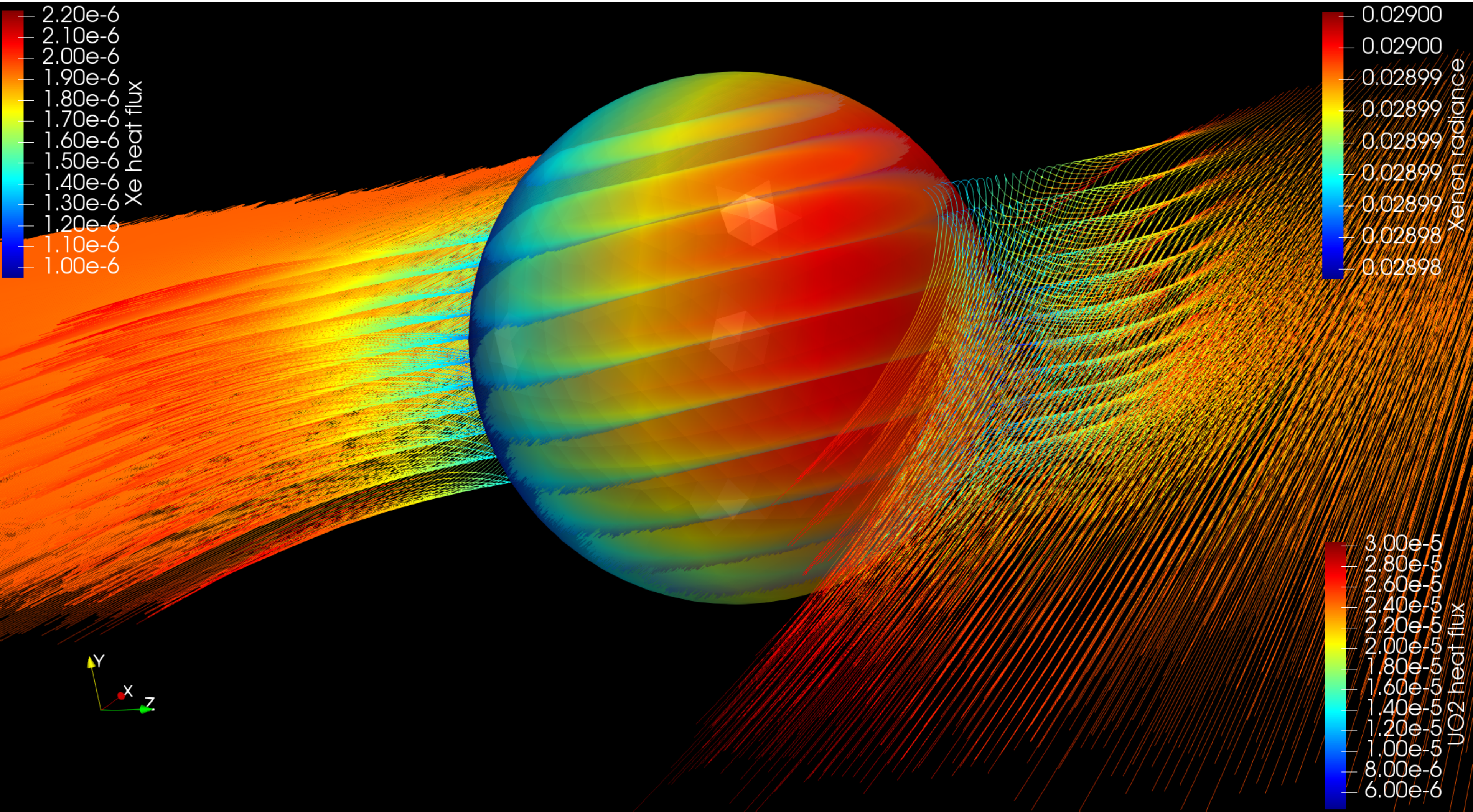
Phonon transport in UO_2 with Xe

- Simulation of uranium dioxide with xenon atoms combining to form a bubble
- Investigating how phonons collide with xenon and scatter, affecting heat transport in the vicinity of the xenon
- Much work has been performed by leveraging geometric artifacts to tune the way heat moves
- How do we set this up?
- Material properties provided by Dr. Laura Rita de Sousa Oliveira of University of Wyoming



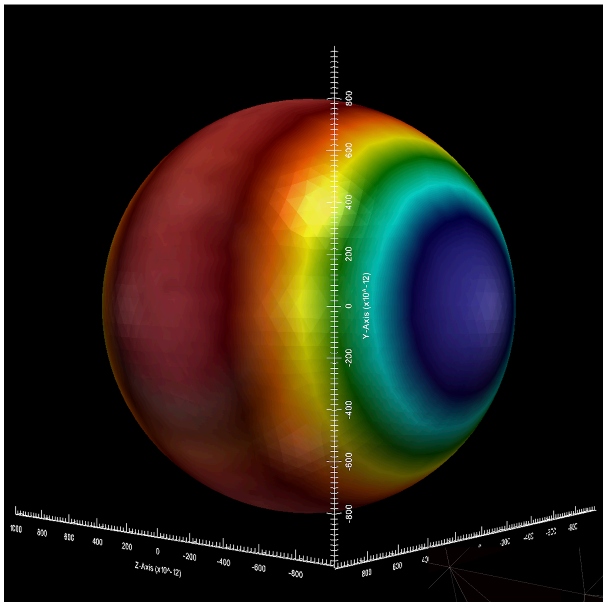
Thermal interfacial resistance

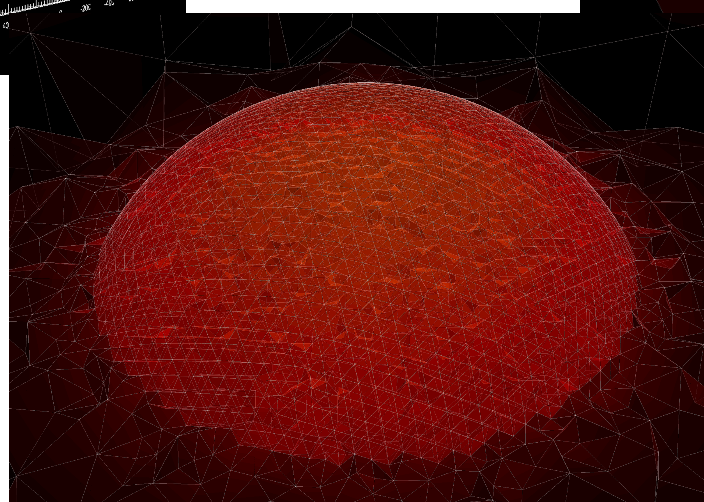
Phonon scattering at UO_2 – Xe interface

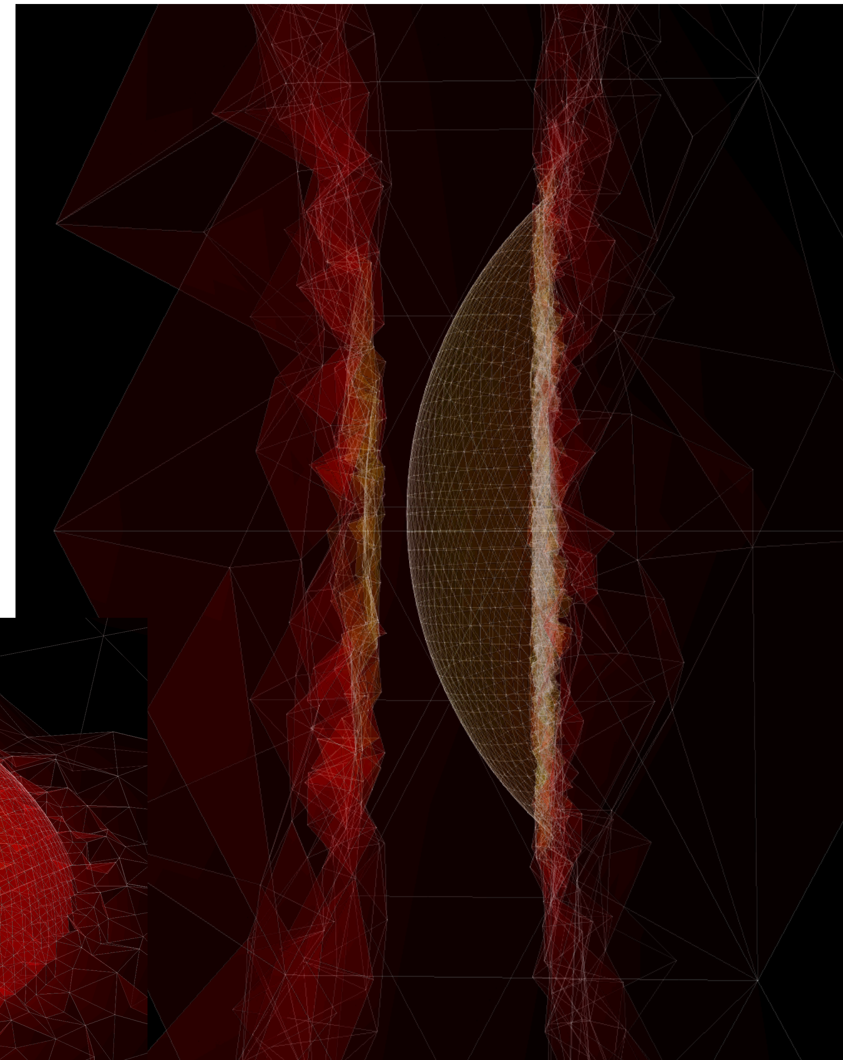


Thermal interfacial resistance

Phonon scattering at UO_2 – Xe interface



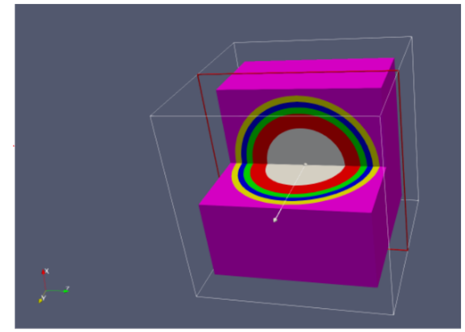


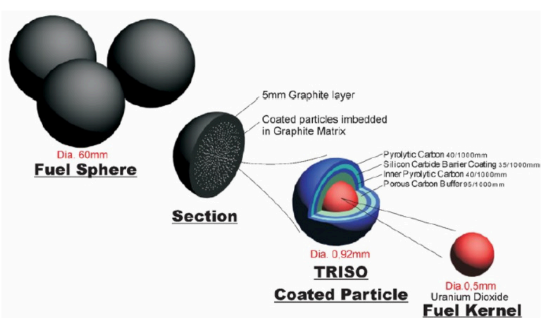


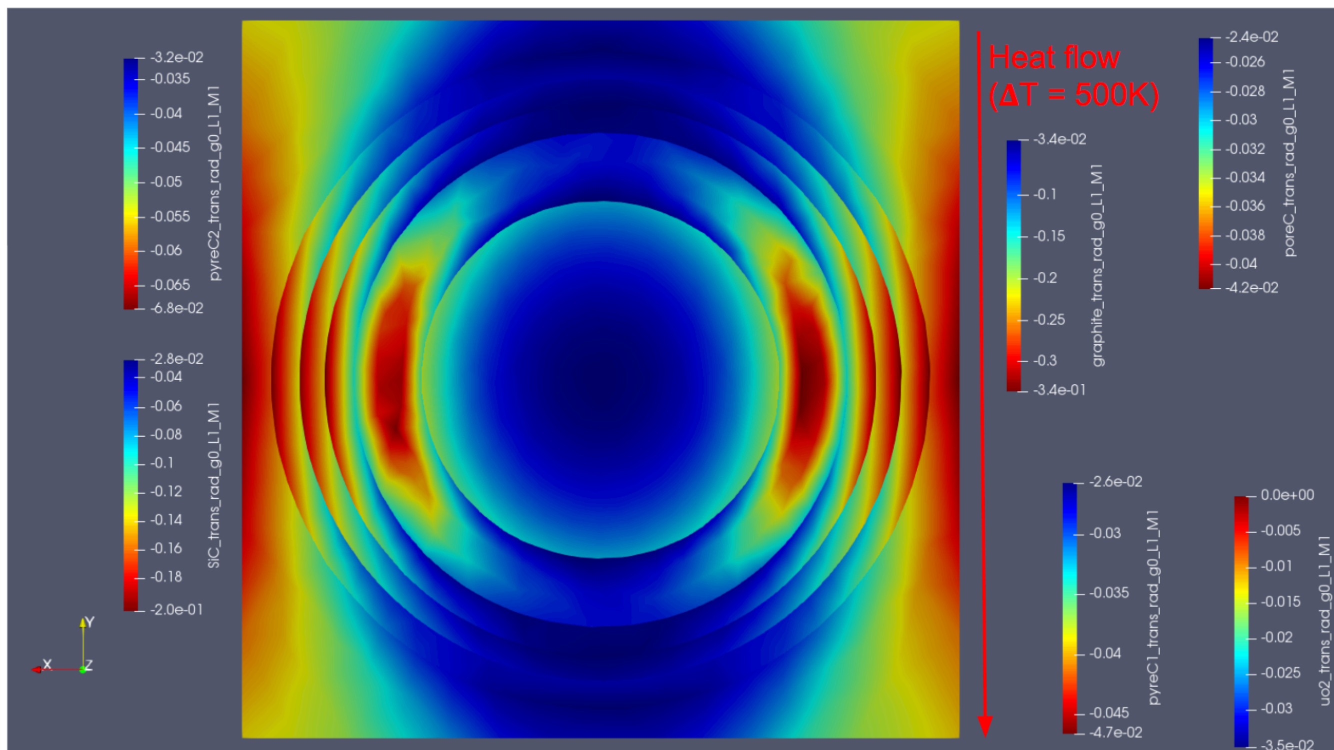
Thermal interfacial resistance

Layered structures (2D/3D)

- Example: TRIstructural ISOtropic (TRISO) fuel kernel. 5 layers, UO_2 kernel in center and layers of pyrolytic carbon, silicon carbide, porous graphite to protect against release of fission products



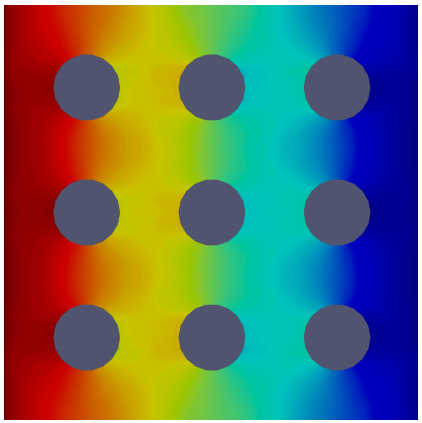


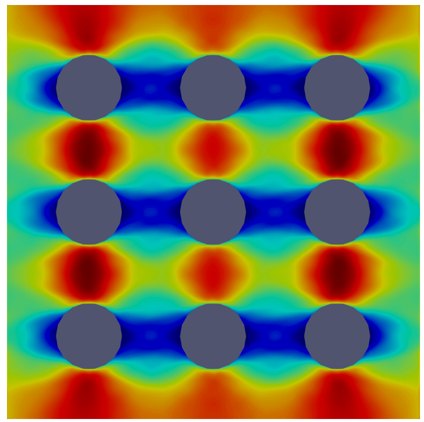


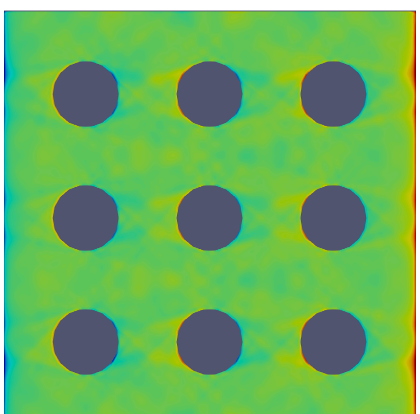
Explicit geometric simulation

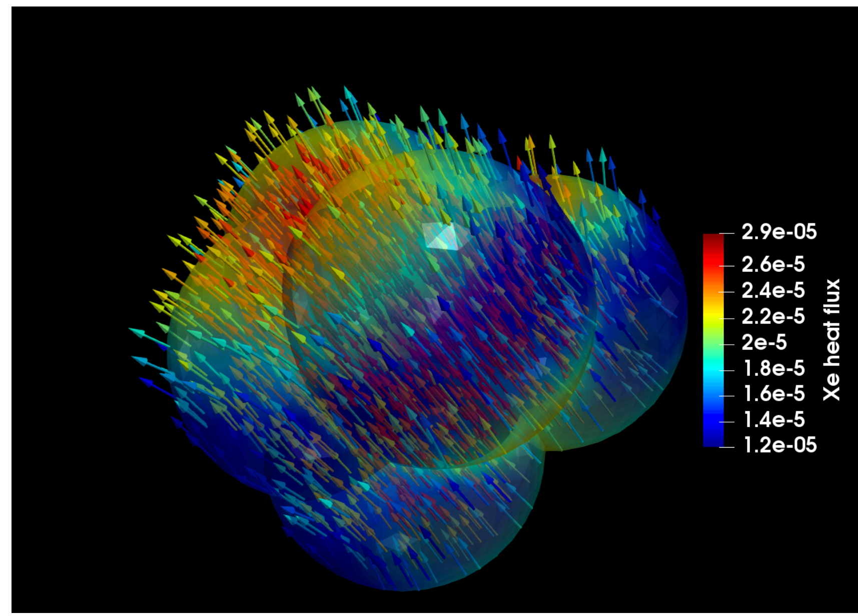
Porous structures or bubbles (2D/3D)

- Example: Si, explicit modeling of pores



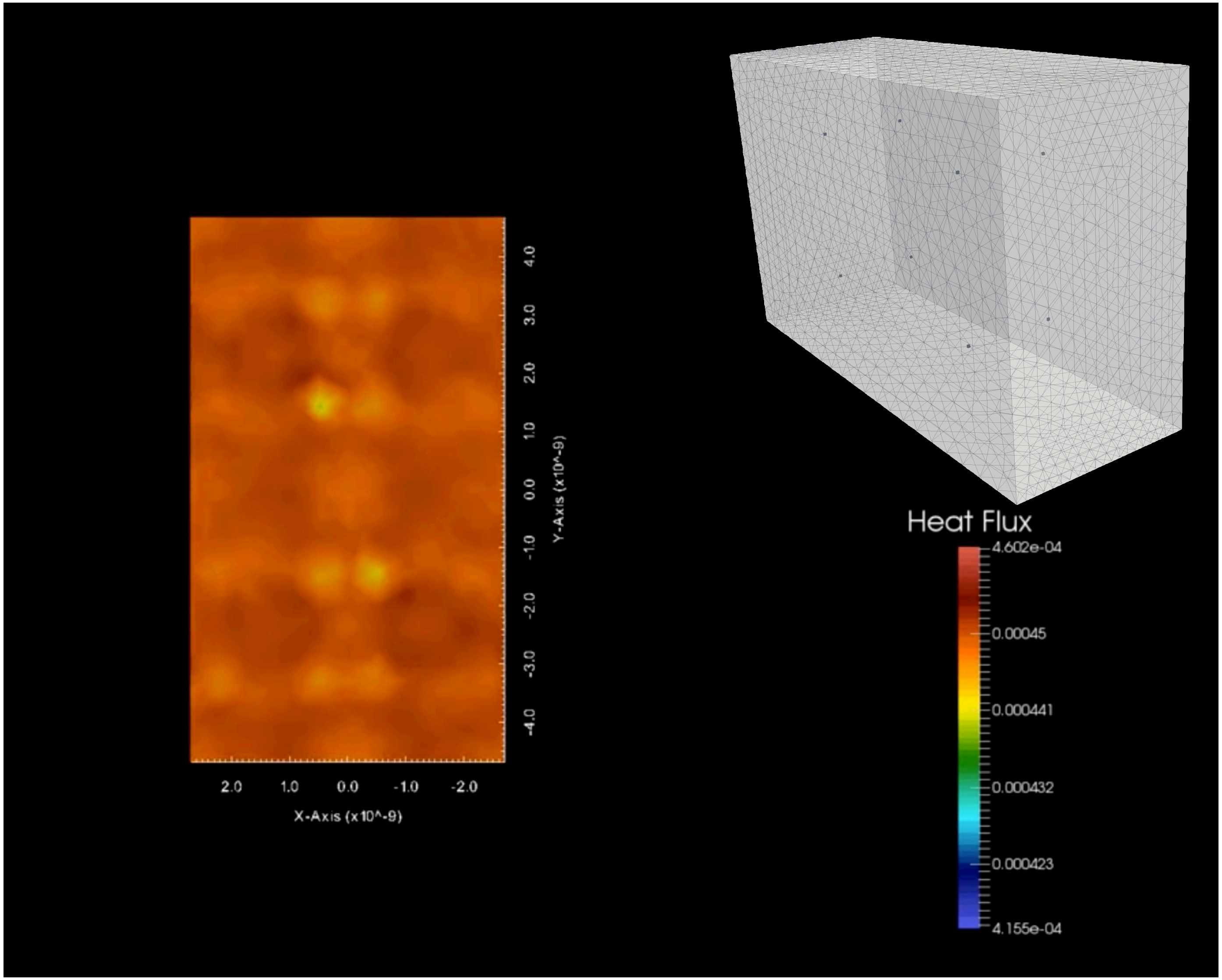




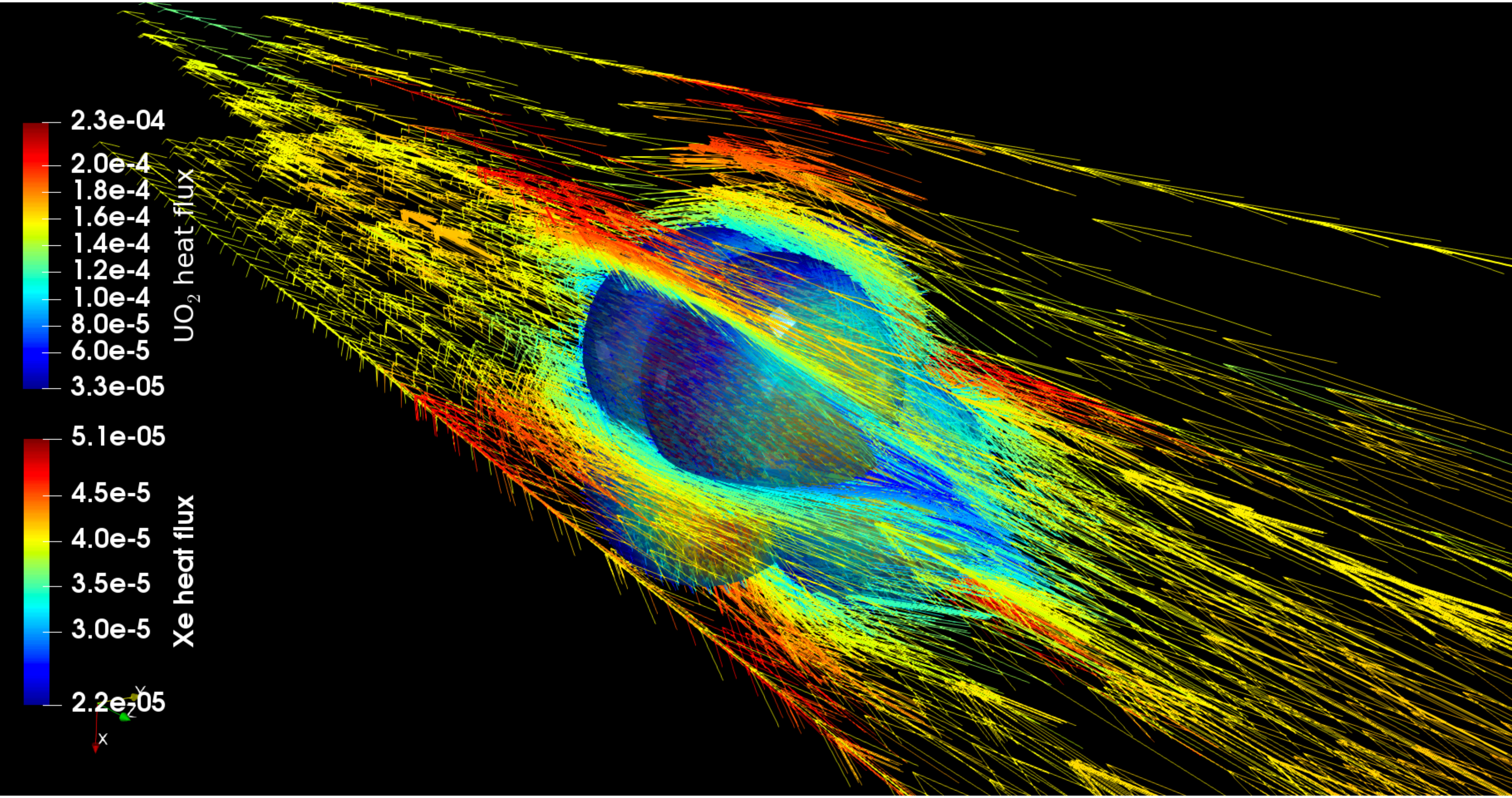


- Example: UO_2 with Xe superstructure
- Heat current prediction

Heat flux fly-by in graphite with carbon defects



Heat flux vorticity in UO_2 with Xe



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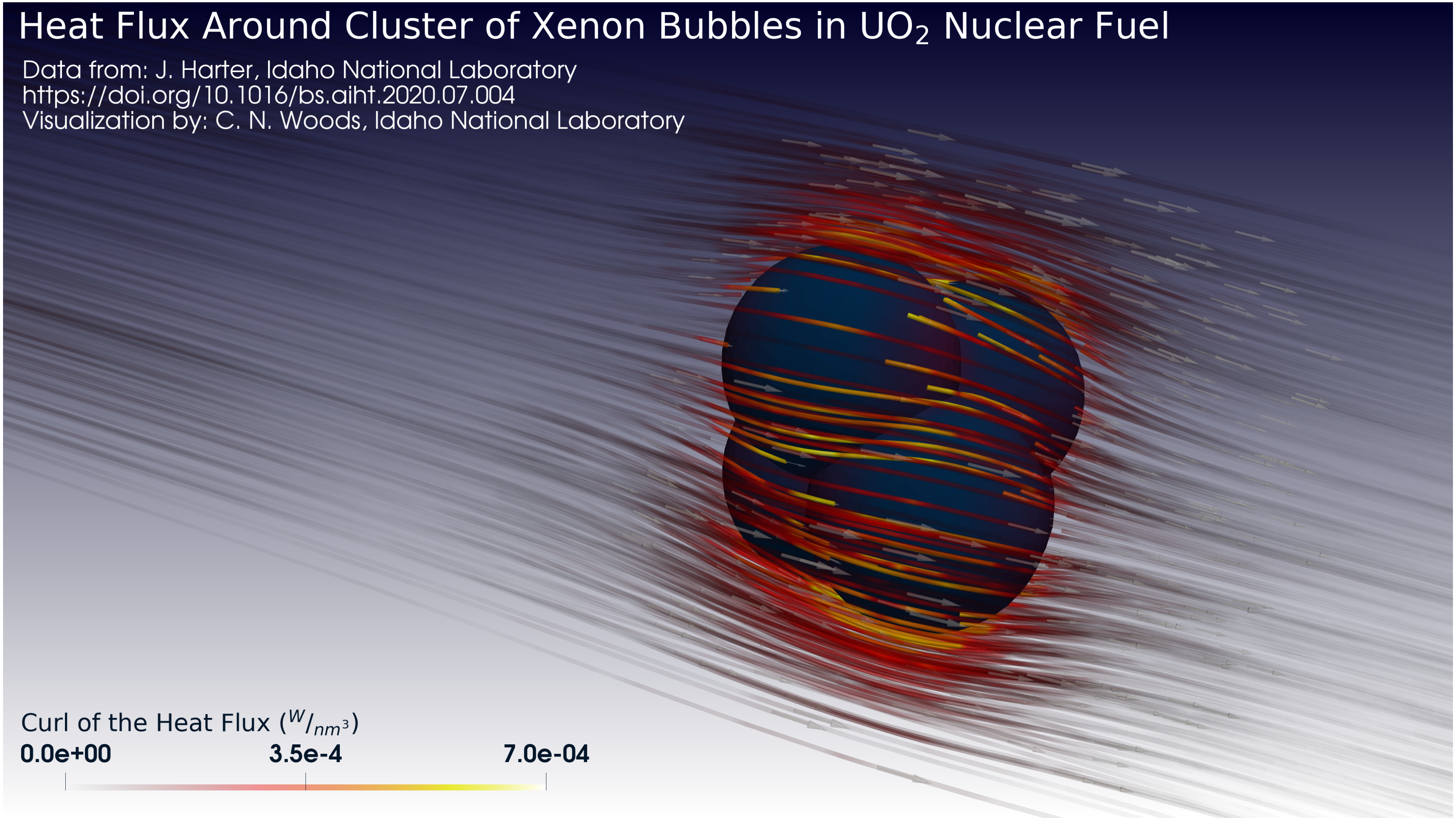
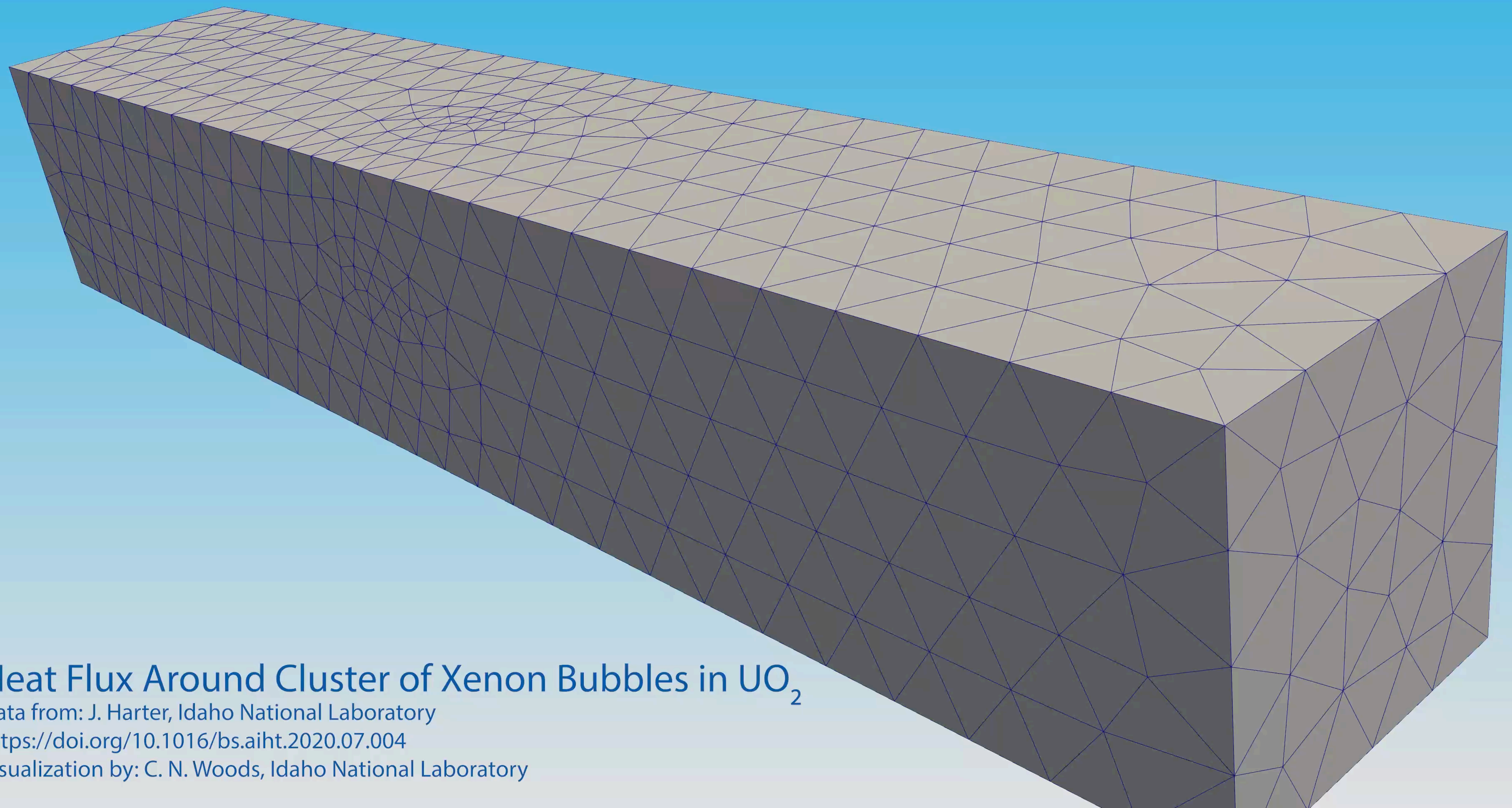


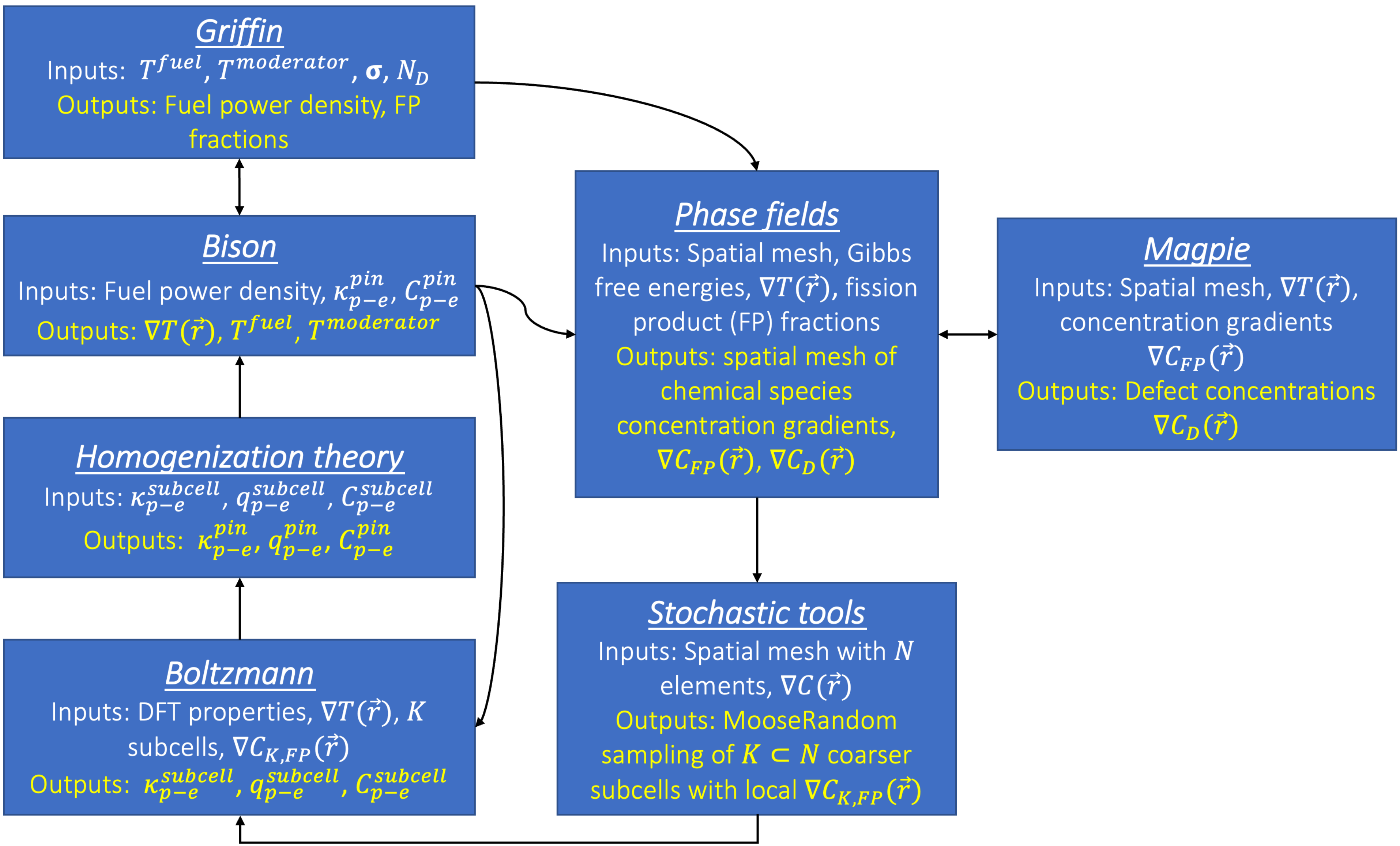
Heat flux vorticity in UO_2 with Xe



Heat Flux Around Cluster of Xenon Bubbles in UO_2
Data from: J. Harter, Idaho National Laboratory
https://doi.org/10.1016/bs.aiht.2020.07.004
Visualization by: C. N. Woods, Idaho National Laboratory

Precision multiscale, multiphysics methods

- The nuclear industry has relied on correlations and empirical fitting for decades to perform its tasks. The result?
  - Large uncertainty prompts enormous conservatism
    - Nuclear cross sections
    - Thermal conductivity
    - Spatial temperature distribution
    - Radiation damage effects
    - Creep and mechanical degradation
  - Why?
  - What do these phenomena have in common?
- What is meant by “precision multiscale”?
  - Escape correlations, empiricism
- How do we model effects in a nuclear fuel pellet?


Griffin
Inputs: T^{fuel}, $T^{moderator}$, $\boldsymbol{\sigma}$, N_D
Outputs: Fuel power density, FP fractions
Bison
Inputs: Fuel power density, κ_{p-e}^{pin}, C_{p-e}^{pin}
Outputs: $\nabla T(\vec{r})$, T^{fuel}, $T^{moderator}$
Homogenization theory
Inputs: $\kappa_{p-e}^{subcell}$, $q_{p-e}^{subcell}$, $C_{p-e}^{subcell}$
Outputs: κ_{p-e}^{pin}, q_{p-e}^{pin}, C_{p-e}^{pin}
Boltzmann
Inputs: DFT properties, $\nabla T(\vec{r})$, K subcells, $\nabla C_{K,FP}(\vec{r})$
Outputs: $\kappa_{p-e}^{subcell}$, $q_{p-e}^{subcell}$, $C_{p-e}^{subcell}$
Phase fields
Inputs: Spatial mesh, Gibbs free energies, $\nabla T(\vec{r})$, fission product (FP) fractions
Outputs: spatial mesh of chemical species concentration gradients, $\nabla C_{FP}(\vec{r})$, $\nabla C_D(\vec{r})$
Magpie
Inputs: Spatial mesh, $\nabla T(\vec{r})$, concentration gradients $\nabla C_{FP}(\vec{r})$
Outputs: Defect concentrations $\nabla C_D(\vec{r})$
Stochastic tools
Inputs: Spatial mesh with N elements, $\nabla C(\vec{r})$
Outputs: MooseRandom sampling of $K \subset N$ coarser subcells with local $\nabla C_{K,FP}(\vec{r})$

Precision multiscale, multiphysics methods

- The answer? Elegant computational science
- HPC resources exist now
  - GPU
  - Artificial intelligence
  - Machine learning
  - Uncertainty Quantification
- What does the new "normal" look like?
  - Past: 1D, 2D, limited 3D nuclear reactor simulations
  - "Curse of dimensionality"
  - Full 3D reactor physics
- J. R. Harter, "White paper: *A comprehensive method for morphological-informed thermal property prediction in the engineering domain*," Tech. Rep. MIS-22-02732, Reactor Physics Methods and Analysis, Idaho National Laboratory, Idaho Falls, Idaho, October 2022

Conclusions

- Microscale heat transfer bridges the gap between the very small and very large
- In the next 10 years…
  - Extreme growth potential
    - Fundamental science
    - Computational and theoretical methods
    - Basic Energy Science (BES), National Science Foundation (NSF), Nuclear Engineering University Partnerships (NEUP), and more…
- How can we change the game?
  - We do the opposite of the current strategy
    - No correlation, no empiricism
    - Full 3D core models with multiphysics
    - Take advantage of the hardware and software tools we have
    - Uncertainty quantification
    - Validate, validate, validate

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