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Poster for LDRD poster presentations

October 2021

Changing the World's Energy Future

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Idaho National Laboratory

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Multiscale thermal properties prediction in the Multiphysics Object Oriented Simulation Environment (MOOSE) via a general Boltzmann solver

(1.2) Transformational Approaches to Accelerate Nuclear RD&D

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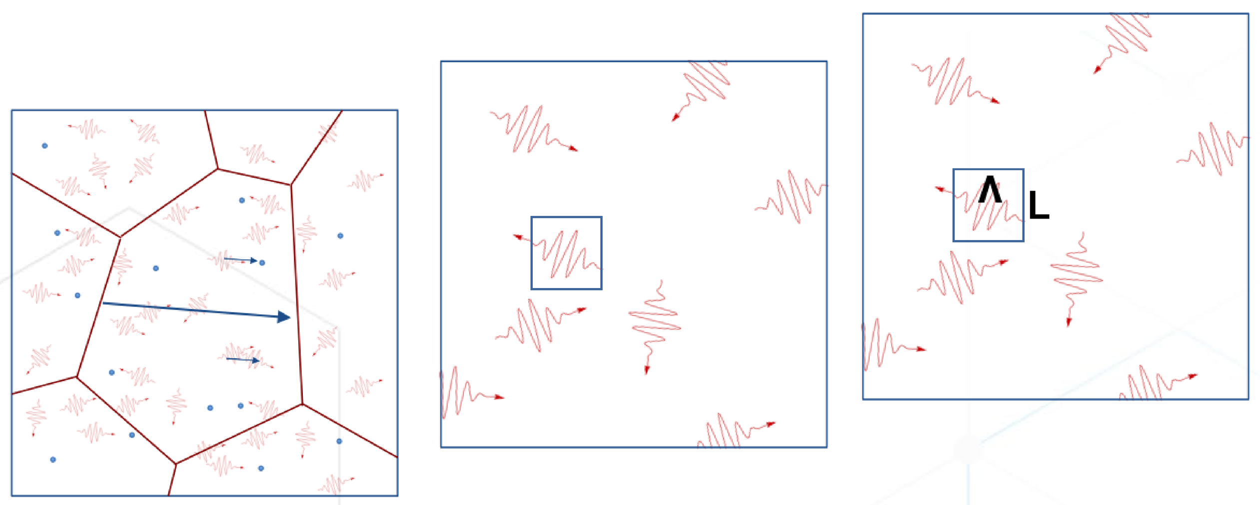
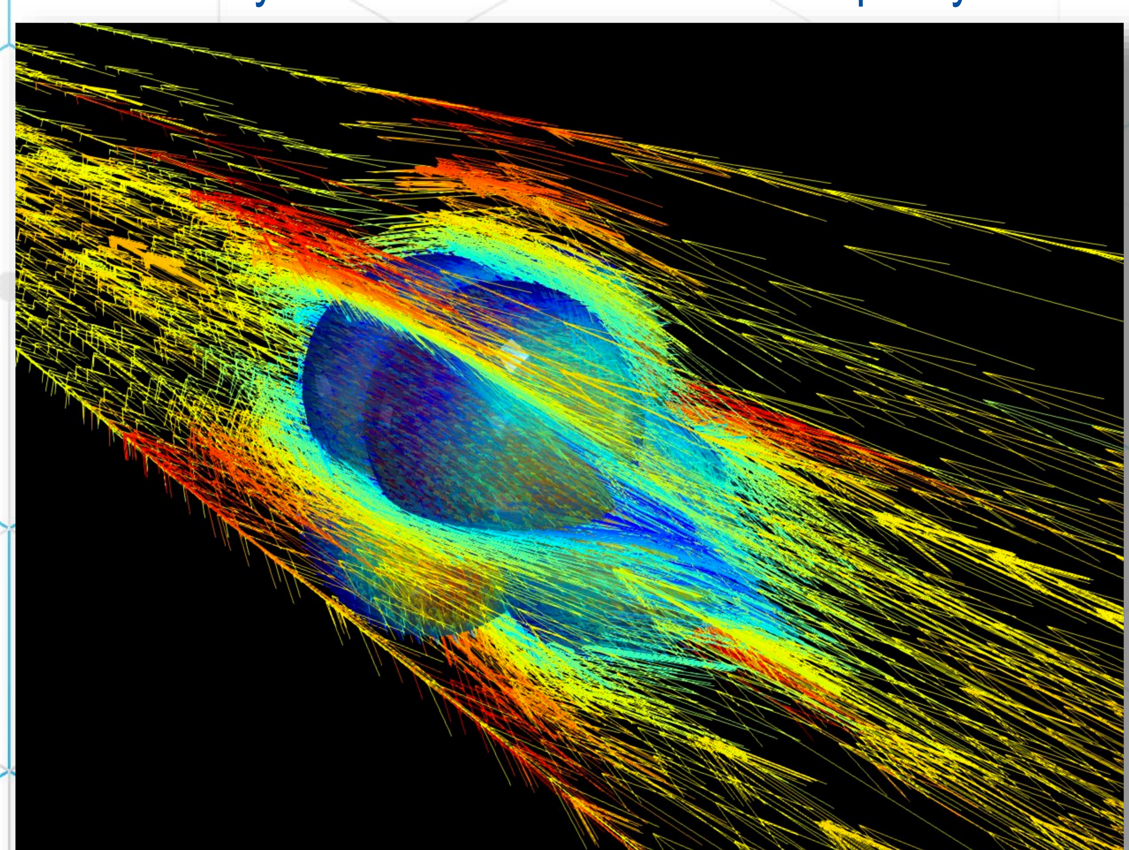
Project Objectives

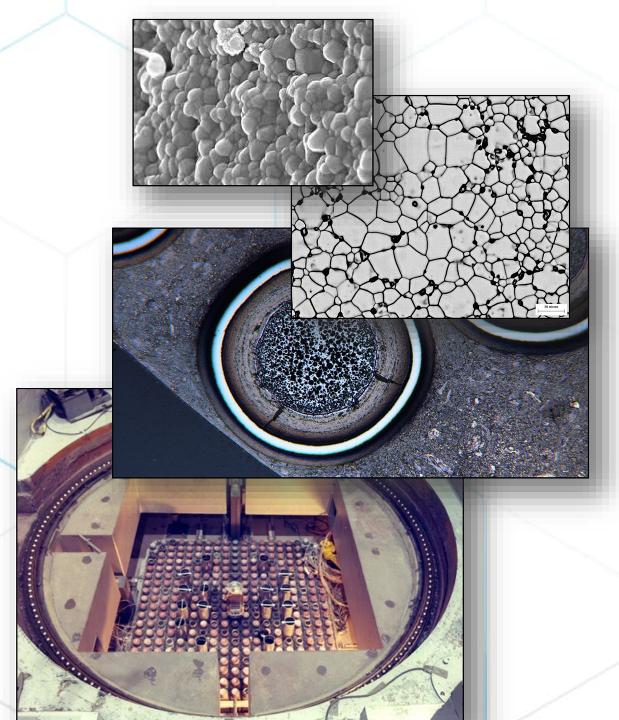
- Engineering-scale fuel performance modeling relies on accurate thermal properties
- Thermal properties are inherently multi-scale, arising from atomistic processes and interactions with a material's microstructure
- Heat transport in solids via conduction occurs through transport and scattering of electrons and phonons



- Use the Boltzmann transport equation (BTE) to predict the macroscopic behavior of a materials system in terms of the microscopic dynamics of its heat carriers



Heat flow around a cluster of Xe bubbles in a UO_2 lattice

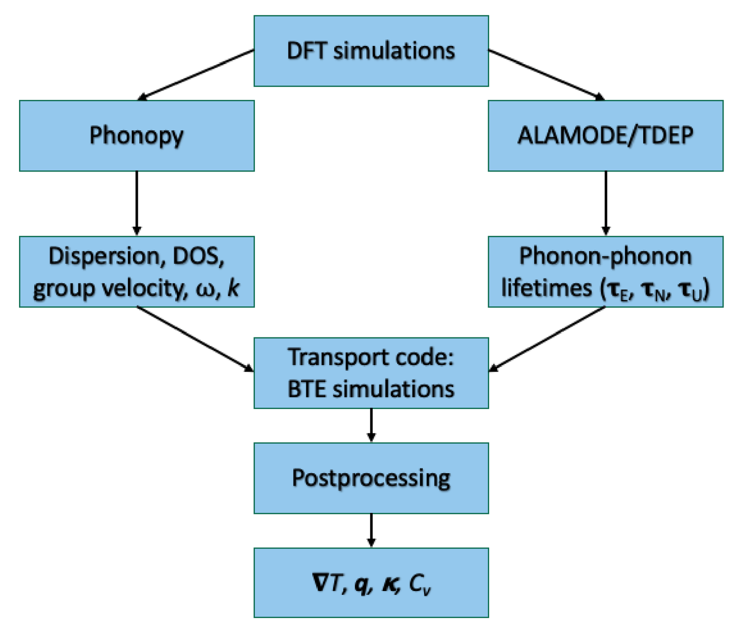


Simulation of fuel performance require physics knowledge on multiple length scales, e.g. TREAT fuel

- This project establishes a new MOOSE (Multiphysics Object Oriented Simulation Environment) module, *Boltzmann*, dedicated to phonon and thermal electron transport

Approach

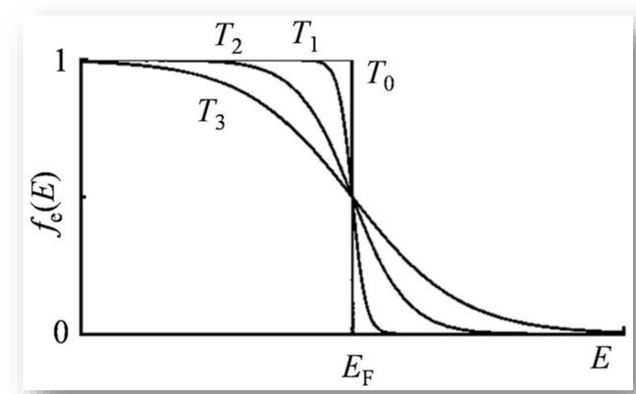
- Providing multigroup (in energy) thermal electron transport is novel, skipping nonlinear solve in temperature
- In transport, thermal electron groups are described by their energy relation to the Fermi level



$$\rho C_p \frac{\partial T}{\partial t} - \vec{\nabla} \cdot \kappa \vec{\nabla} T$$

$$\kappa = -\frac{q(r)}{\nabla T(r)}$$

$$\kappa = \frac{1}{3} C_p v^2 \tau$$



- Use *modified source iteration*, perform additional analytical steps linking energy groups together via temperature and Fermi energy

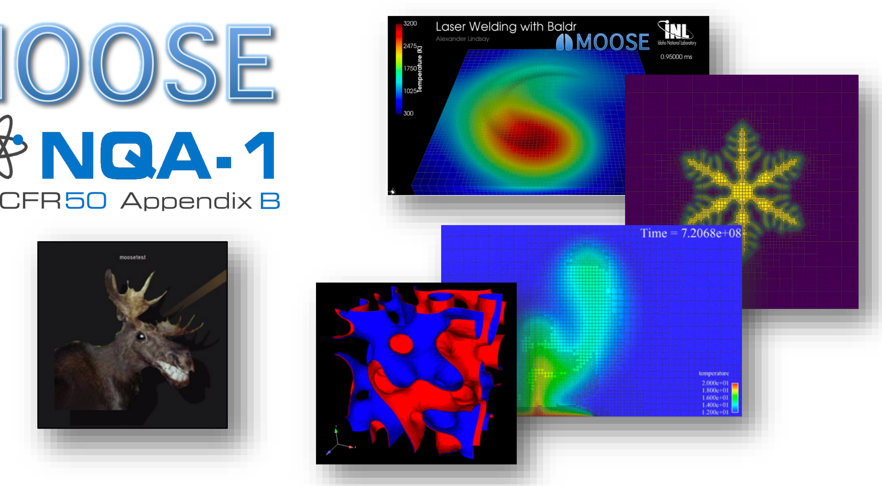
$$v(\mathbf{k})\,\hat{\boldsymbol{\Omega}} \cdot \nabla_{\mathbf{r}} f\left(\mathbf{r}, \hat{\boldsymbol{\Omega}}, E\right) = \frac{f^{\mathrm{FD}}\left(T(\mathbf{r}), E, E_{\mathrm{F}}\right) - f\left(\mathbf{r}, \hat{\boldsymbol{\Omega}}, E\right)}{\tau(\mathbf{k})}$$

- Use Fermi-Dirac (FD) statistics as a source term
- Main challenge is developing the intermediate step to solve for temperature and Fermi energy, interdependent quantities

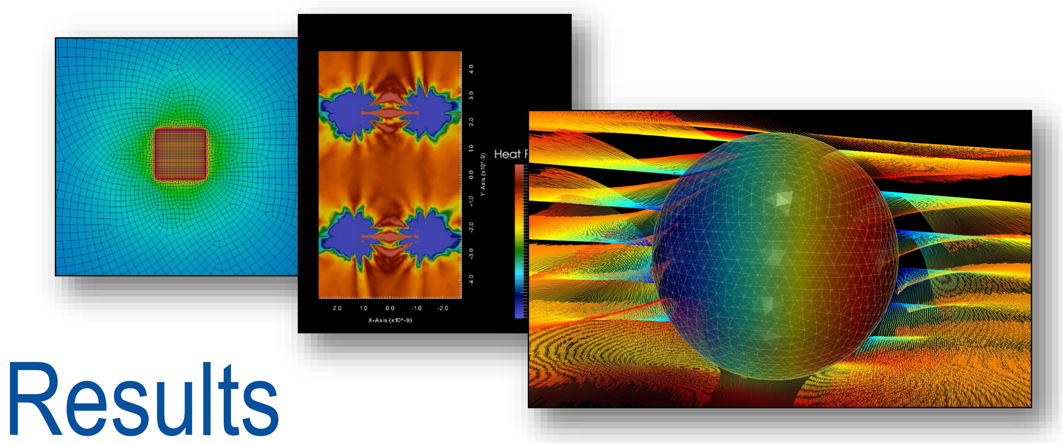
Novelty

- MOOSE developed to NQA-1 (Nuclear Quality Assurance) standards, constantly evolving, seamlessly incorporates complimentary physics

MOOSE NQA-1 10CFR50 Appendix B



- Coupling thermal electron groups using FD statistics not currently implemented elsewhere
- Flexible finite element framework



Results

We are in the final stages of implementing of the thermal electron transport code. The phonon transport code exists in the *Griffin* particle transport suite and will be migrated to the *Boltzmann* module. An invited book chapter, "*Predicting mesoscale spectral thermal conductivity using advanced deterministic phonon transport techniques*", was published in the series *Advances in Heat Transfer*, Vol. 52, 2020, pp. 335-482.

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