Fully-coupled engineering and mesoscale simulations of thermal conductivity in UO$_2$ fuel using an implicit multiscale approach

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Abstract. Though the thermal conductivity of solid UO$_2$ is well characterized, its value is sensitive to microstructure changes. In this study, we propose a two-way coupling of a mesoscale phase field irradiation model to an engineering scale, finite element calculation to capture the microstructure dependence of the conductivity. To achieve this, the engineering scale thermomechanics system is solved in a parallel, fully-coupled, fully-implicit manner using the preconditioned Jacobian-free Newton Krylov (JFNK) method. Within the JFNK function evaluation phase of the calculation, the microstructure-influenced thermal conductivity is calculated by the mesoscale model and passed back to the engineering scale calculation. Initial results illustrate quadratic nonlinear convergence and good parallel scalability.

1. Introduction
Thermal conductivity of UO$_2$ fuel in a light water reactor strongly impacts both the design of the fuel and the operation of the reactor system employing it. As the fuel undergoes irradiation, the temperature and neutron flux gradients cause fission products and porosity to form within the pellet. Microstructure evolution results in different local thermal conductivities throughout the fuel pellet. Rokkam et al.[1] have developed a mesoscale phase field model that predicts the nucleation and growth of voids due to irradiation. The microstructure predicted by the method can then be used to calculate an effective thermal conductivity [2]. However, the computational expense of modeling the entire fuel pellet with such a mesoscale model would be prohibitively large.

To investigate the impact of a microstructurally-dependent thermal conductivity on engineering scale thermomechanics, this study proposes an approach to couple an engineering scale calculation with a mesoscale phase field calculation. Fully coupled multiscale calculations are challenging due to operator splitting and extreme diversity in both spatial and temporal scales. To address both of these considerations, the nonlinear engineering scale calculation is consistently coupled with the mesoscale solution and then solved using a preconditioned Jacobian-free Newton Krylov (JFNK) [3] method. In this paper, we describe our initial approach to a multiscale model of a UO$_2$ fuel pellet. Section 2 briefly summarizes the engineering scale and mesoscale models and discusses the scale bridging method. In section 3, initial results from the multiscale model are presented.
2. The multiscale model

Typically, thermal conductivity impacts heat conduction within the fuel according to

\[
\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot q - Q = 0 \quad T \in \Omega,
\]

\[
\mathbf{n} \cdot \mathbf{q} = q(T) \quad T \in \Gamma^T, \Gamma^B.
\]

\[
\mathbf{n} \cdot \mathbf{q} = 0 \quad T \in \Gamma^C \cup \Gamma^B,
\]

\[
T(t = 0) = T_0 \quad T \in \Omega,
\]

where \(T, \rho\) and \(C_p\) are temperature, density and specific heat of UO\(_2\), respectively, and we assume fission reactions generate heat at a uniformly distributed constant rate \(Q\). In this expression, \(\Gamma^T\) denotes the top, \(\Gamma^B\) denotes the bottom and \(\Gamma^C\) denotes the outer circumferential boundaries of the fuel pellet such that \(\Gamma = \Gamma^T \cup \Gamma^B \cup \Gamma^C\), and \(q(T)\) is an expression of the heat rejected to the cladding. The heat flux \(q\) within the UO\(_2\) domain \(\Omega\) may be written as \(q = -k \nabla T\), where \(k\) is the thermal conductivity of UO\(_2\), assuming that the transfer of mass due to species diffusion is small.

In a fuel pellet undergoing irradiation within a reactor, the values of \(k, \rho,\) and \(C_p\) depend on the microstructure of the material, including voids and fission products, though in this work we only consider the microstructure effect on \(k\). In our multiscale simulations, the heat flux problem is solved by the engineering scale model, while the value of \(k\) is determined by the mesoscale model.

2.1. Engineering (coarse) scale discretization

The engineering scale model is a fully-coupled finite element implementation of Eq. (1) with a linear mechanics model of a UO\(_2\) fuel pellet [4]. The coarse test space \(V\) is approximated by \(V^h\) using linear Lagrange finite elements such that \(V^h \subset V\) and \(V^h = \text{span}\{\phi_i\}_{i=1}^n\). The trial space hosting the engineering scale solution is similarly approximated, where \(T \in V^h\) is

\[
T(t, \mathbf{x}) = \sum_{j=1}^n T_j(t) \phi_j(\mathbf{x}).
\]

The model is implemented in Idaho National Laboratory’s BISON fuel performance code. BISON is built upon INL’s MOOSE: a parallel, nonlinear, computational framework [5].

In our calculations, we employ Eq. (1) in weak form from Newman et al.[4]. The JFNK solution method used in BISON begins with casting this weak form solution as a residual function, i.e.

\[
\mathbf{F}(\mathbf{x}) = 0
\]

of length \(N\), where \(N\) is the number of unknowns in the discrete problem. The Jacobian of this system is a \(N \times N\) sparse matrix,

\[
\mathbf{J}(\mathbf{x}) = \frac{\partial \mathbf{F}(\mathbf{x})}{\partial \mathbf{x}},
\]

where the components of \(\mathbf{F}(\mathbf{x})\) are taken directly from the weak form of the problem. Given the Jacobian and the outline in Newman et al.[4], one can express Newton’s method in terms of the solution of a series of linear systems. In right preconditioned form, these linear systems may be written as

\[
\mathbf{J}(\mathbf{x}^{(k)}) M^{-1}(M \delta \mathbf{x}^{(k)}) = -\mathbf{F}(\mathbf{x}^{(k)}),
\]

where \(M^{-1}\) symbolically represents the preconditioning process.
two stable phases; \( c \) where \( < \) defined by the continuous order parameter \( \eta \). In addition, we evolve the microstructure within a 2D domain. In the model, the vacancies are defined by a conserved concentration field \( c_v \) and the void phase is defined by the continuous order parameter \( \eta \) in a solid material and \( \eta = 1 \) in a void. The void and vacancy behavior is defined by a free energy function with two energy wells defining two stable phases; \( \eta = 0 \) and \( c_v = c_{v0} \) and the void phase (\( \eta = 1 \) and \( c_v = 1 \)), where \( c_{v0} = c_v^0 \exp(-E_v^m/k_BT) \) is the vacancy equilibrium concentration with Boltzmann constant \( k_b \).

The evolution of \( c_v \) and \( \eta \) is defined by

\[
\frac{\partial c_v}{\partial t} = \nabla \cdot M_v \nabla \frac{1}{N} \frac{\partial F(c_v, \eta)}{\partial c_v} \tag{6}
\]

\[
\frac{\partial \eta}{\partial t} = -\frac{1}{N} L_v \frac{\partial F(c_v, \eta)}{\partial \eta}, \tag{7}
\]

where \( M_v = D_v/(k_b T) \) is the vacancy mobility with the diffusivity \( D_v = D_v^0 \exp(E_v^m/k_BT) \), and \( L_v \) is the order parameter mobility. To model the irradiation, there is a probability \( P_{\text{casc}} \) that \( c_v \) will increase by a random amount up to the maximum value \( c_{\text{max}} \).

For this work, Eqs. (6) and (7) are uniformly discretized in space and solved using an explicit finite-difference approach with forward Euler time-stepping. Once the microstructure has evolve for a specified amount of time at a uniform temperature, the spatially-dependent mesoscale thermal conductivity is calculated void formation over the fine space, resulting in the spatially-dependent mesoscale thermal conductivity \( k'(\mathbf{r}) \) defined in the previous section. However, the coarse space does not resolve this mesoscale spatial dependence. We determine the coarse space thermal conductivity \( k \) by solving a

\[\begin{array}{cccccccccc}
D_v^0 & c_v^0 & E_v^m & E_v^f & L_v & A & B & \kappa_v & \kappa_\eta & P_{\text{casc}} & c_{\text{max}} \\
1643.0 \text{ a.u.} & 1.0 & 1.0 \text{ eV} & 1.0 \text{ eV} & 1 & 1 \text{ eV} & 1 \text{ eV} & 0.5 \text{ eV/nm}^2 & 1.0 \text{ eV/nm}^2 & 0.3\% & 1.0
\end{array}\]

### Table 1. Values for the mesoscale model parameters. The diffusivity is in arbitrary units (a.u.). See Rokkam et al.[1] for the meaning of each parameter.

2.2. Mesoscale (fine) scale simulation

To simulate the microstructure evolution due to irradiation in the UO\(_2\) fuel, we employ the phase field model developed in Rokkam et al.[1]. The model for this preliminary study represents a simplified description of the fuel, since it only considers vacancies and assumes the material is comprised of a single component. In addition, we evolve the microstructure within a 2D domain.

In the model, the vacancies are defined by a conserved concentration field \( c_v(\mathbf{r}, t) \) and the void phase is defined by the continuous order parameter \( \eta(\mathbf{r}, t) < 1 \), where \( \eta = 0 \) in a solid material and \( \eta = 1 \) in a void. The void and vacancy behavior is defined by a free energy function with two energy wells defining two stable phases; \( \eta = 0 \) and \( c_v = c_{v0} \) and the void phase (\( \eta = 1 \) and \( c_v = 1 \)), where \( c_{v0}^\text{eq} = c_v^0 \exp(-E_v^m/k_BT) \) is the vacancy equilibrium concentration with Boltzmann constant \( k_b \).

The evolution of \( c_v \) and \( \eta \) is defined by

\[
\frac{\partial c_v}{\partial t} = \nabla \cdot M_v \nabla \frac{1}{N} \frac{\partial F(c_v, \eta)}{\partial c_v} \tag{6}
\]

\[
\frac{\partial \eta}{\partial t} = -\frac{1}{N} L_v \frac{\partial F(c_v, \eta)}{\partial \eta}, \tag{7}
\]

where \( M_v = D_v/(k_b T) \) is the vacancy mobility with the diffusivity \( D_v = D_v^0 \exp(E_v^m/k_BT) \), and \( L_v \) is the order parameter mobility. To model the irradiation, there is a probability \( P_{\text{casc}} \) that \( c_v \) will increase by a random amount up to the maximum value \( c_{\text{max}} \).

For this work, Eqs. (6) and (7) are uniformly discretized in space and solved using an explicit finite-difference approach with forward Euler time-stepping. Once the microstructure has evolve for a specified amount of time at a uniform temperature, the spatially-dependent mesoscale thermal conductivity is defined as \( k'(\mathbf{r}) = k_{\text{bulk}} \) if \( \eta \leq 0.8 \) and \( k'(\mathbf{r}) = k_{\text{void}} \) if \( \eta > 0.8 \). We assume the void conductivity to be that of He gas, \( k_{\text{void}} = 0.152 \text{ W/m K} \), and we use the temperature-dependent expression for \( k_{\text{bulk}} \) in UO\(_2\) from Lucuta et al.[6]. Table 1 summarizes the parameter values for the mesoscale model used in this work.

2.3. Scale bridging

There is a disparity between the spatial and time scales in the mesoscale and engineering scale models. To couple the two models, we must bridge the scales.

While the engineering scale model may take time steps of hours or days, the mesoscale model requires much smaller time steps. We bridge the time scale in a similar manner to accelerated experimentation techniques, \textit{i.e.} a much higher irradiation rate is considered at the mesoscale. Therefore, the amount of time required to reach a specified burnup is different at the two scales. This approach does introduce some error into the calculation, since the diffusivity is equal in both time scales.

The spatial bridging method employed here is similar to the method proposed by Wagner and Liu [7]. We define coarse and fine calculational spaces, where the coarse space spans the complete problem geometry and the fine space exists only at the Gauss points on the engineering mesh. The mesoscale model calculates void formation over the fine space, resulting in the spatially-dependent mesoscale thermal conductivity \( k'(\mathbf{r}) \) defined in the previous section. However, the coarse space does not resolve this mesoscale spatial dependence. We determine the coarse space thermal conductivity \( k \) by solving a
steady-state conductivity equation [2],

\[ \nabla \cdot (k'(r)\nabla T) = 0, \]  

in the fine space using the evolved microstructure. Equation (8) is discretized and solved using the same grid as that used for the phase field simulations. A constant-temperature boundary condition of \( T_l = 800 \) K is applied on the left boundary and a constant heat flux of \( q' = 50 \text{ MW/m}^2 \) is applied across the right boundary; periodic boundary conditions are applied in the \( y \)-direction (note that the values of \( T_l \) and \( q' \) are arbitrarily selected and have no effect on the value of the calculated thermal conductivity). Assuming \( q = q' \), \( k \) is determined with \( q = -k\Delta T \), where \( \Delta T \) is the difference between the temperature on the left boundary of the fine space \( (T_l = 800 \text{ K}) \) and the average temperature on the right boundary.

The microstructure predicted by the mesoscale model is random, due to the random irradiation term. However, the engineering scale should not resolve this mesoscale randomness. To determine a mesoscale grid size for which the random variation of \( k \) is sufficiently small, we calculate \( k \) at 20 temperatures within the narrow range \( 999.9 \leq T \leq 1000.1 \). We repeat the calculation for increasing grid sizes ranging from \( 128 \times 128 \) to \( 1024 \times 1024 \) and calculate the standard deviation of the random scatter (see Fig. 1(a) for the standard deviations from various grid sizes). The standard deviation decreases with increasing grid size, but even at a grid size of \( 1024 \times 1024 \), some random variation is still apparent.

The mesoscale grid size required to eliminate the randomness from the macroscale \( k \) would be computationally prohibitive in the multiscale model. To allow for small grid sizes, we employ a dynamic curve fitting method to bridge the length scale. Using a least mean squares algorithm, we fit all the values of \( k \) calculated by the mesoscale model with a fourth-order polynomial. The thermal conductivity used by the engineering scale model is taken from the curve fit, while the values calculated by the mesoscale model are used to refine the fit. The mesoscale model does not calculate a conductivity when the current temperature is within a certain tolerance of a temperature at which \( k \) was previously calculated, and the fit is only recalculated at the start of each residual calculation.

3. Results
Here, we calculate the temperature distribution in a \( \text{UO}_2 \) fuel pellet. The purpose of this simulation is a proof-of-concept of our multiscale model, not to accurately predict the thermal behavior in a \( \text{UO}_2 \) pellet. Therefore, we make several assumptions to simplify the calculation.

We consider a dished \( \text{UO}_2 \) pellet of radius \( r = 4.13 \) mm and height \( h = 6.75 \) mm. The pellet has a constant temperature boundary condition \( T_c = 700 \) K on the outer circumference and a heat source of \( Q = 400 \text{ MW/m}^3 \) applied to the pellet. Also, steady-state heat conduction is assumed and the pellet is discretized with 720 linear hexhedral elements. In the mesoscale calculations, we consider a 2D square of \( \text{UO}_2 \) with sides \( l = 1.28 \) \( \mu \)m discretized with a \( 128 \times 128 \) finite difference grid. The parameters from Table 1 are used and the sample is irradiated for 120 arbitrary time units.

The multiscale calculation converged quadratically (see Fig. 1(b)) and it exhibits excellent parallel scalability (Fig. 1(c)). Figures 2(a) and 2(b) show the temperature distribution within the pellet and the dependence of the thermal conductivity \( k \) with temperature, respectively. From plots of the mesoscale vacancy concentration at three positions in the pellet (see Figs. 2(c) – 2(e)), we observe that large voids, surrounded by vacancy-depleted zones, have formed in the center of the pellet. At mid-radius, a larger number of small voids have formed. On the outer circumference, no voids are present.

4. Conclusions
Our multiscale model calculates the temperature distribution in a fuel pellet, considering the microstructure-dependence of the thermal conductivity. The JFNK solution converges quadratically and has excellent parallel scalability. The final microstructure shows strong spatial-dependence.

This work represents a proof-of-concept of our multiscale model. Significant work is still needed to accurately predict the thermomechanical behavior in a \( \text{UO}_2 \) fuel pellet. In future studies, more physics
Figure 1. (a) The standard deviation of the random scatter in the thermal conductivity at increasing grid sizes, (b) the residual value at each of the six JFNK solution iterations and (c) the computation time from different numbers of parallel processors, showing excellent parallel scalability.

![Figure 1](image1.png)

Figure 2. (a) The temperature distribution in the fuel pellet, (b) conductivity vs. temperature from the mesoscale model, (c) - (e) plots of the final $c_v$ at $r = 4.13$ mm, $r = 2.07$ mm and $r = 0.0$ mm, respectively.

![Figure 2](image2.png)

will be incorporated in the mesoscale model (fission gas, multiple components, self-interstitials) which will be evolved on a 3D domain. Furthermore, the engineering scale simulation will be time-dependent rather than steady-state.

References
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