INL/CON-13-28113
PREPRINT

Algorithms for Thermal and Mechanical Contact in Nuclear Fuel Performance Analysis

M&C 2013

J. D. Hales
D. Andrs
D. R. Gaston

May 2013

International Conference on Mathematics and Computational Methods Applied to Nuclear Science & Engineering (M&C 2013)
Sun Valley, Idaho, USA, May 5-9, 2013, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2013)

ALGORITHMS FOR THERMAL AND MECHANICAL CONTACT IN NUCLEAR FUEL PERFORMANCE ANALYSIS

J. D. Hales and D. Andrs and D. R. Gaston
Idaho National Laboratory
2525 N. Fremont Ave, Idaho Falls, ID 82415
jason.hales@inl.gov; david.andrs@inl.gov; derek.gaston@inl.gov

ABSTRACT

The transfer of heat and force from UO_2 pellets to the cladding is an essential element in typical nuclear fuel performance modeling. Traditionally, this has been accomplished in a one-dimensional fashion, with a slice of fuel interacting with a slice of cladding. In this manner, the location at which the transfer occurs is set *a priori*. While straightforward, this limits the applicability and accuracy of the model.

We propose finite element algorithms for the transfer of heat and force where the location for the transfer is not predetermined. This enables analysis of individual fuel pellets with large sliding between the fuel and the cladding.

The simplest of these approaches is a node on face constraint. Heat and force are transferred from a node on the fuel to the cladding face opposite. Another option is a transfer based on quadrature point locations, which is applied here to the transfer of heat. The final algorithm outlined here is the so-called mortar method, with applicability to heat and force transfer. The mortar method promises to be a highly accurate approach which may be used for a transfer of other quantities and in other contexts, such as heat from cladding to a CFD mesh of the coolant.

This paper reviews these approaches, discusses their strengths and weaknesses, and presents results from each on simplified nuclear fuel performance models.

Key Words: nuclear fuel performance modeling, constraint enforcement, mortar method

1. INTRODUCTION

Since 2008, the Idaho National Laboratory (INL) has been developing next-generation capabilities to model nuclear fuel behavior. One such effort has focused on the development of a new multidimensional finite element fuels code called BISON[1]. BISON is written to be a general-use fuels performance analysis tool. While primarily used to analyze UO_2 fuel in Zircaloy cladding, BISON has also been applied to plate fuel, metal fuel and tristructural-isotropic (TRISO) fuel analysis.

Of particular importance in modeling UO_2 fuel is the interaction between the fuel and cladding across a gas-filled gap. Heat transfer across the gap is a vital component of the modeling effort. Later in life, the fuel comes into contact with the cladding, pressing the cladding outward. The treatment of these interactions – gap heat transfer and mechanical contact – is the subject of this paper.

1.1. Thermal and Mechanical Contact Constraints

The heat conduction equation as applied to nuclear fuel is taken as

$$\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot \mathbf{q} - E_f \dot{F} = 0, \tag{1}$$

where T, ρ and C_p are the temperature, density and specific heat, respectively, E_f is the energy released in a single fission event, and $\dot{F}$ is the volumetric fission rate. The heat flux is given as

$$\mathbf{q} = -k\nabla T, \tag{2}$$

where k denotes the thermal conductivity of the material. Heat transfer in the cladding follows the same form minus the source term due to the energy of fission.

Pairing a boundary of the fuel domain with a boundary of the cladding between which heat must be transferred (e.g., the outer radius of the fuel and the inner surface of the cladding), the governing equation is

$$\begin{aligned} \int_{\Gamma_1} \mathbf{n}_1 \cdot \mathbf{q}_1 &= -\int_{\Gamma_2} \mathbf{n}_2 \cdot \mathbf{q}_2 \\ \int_{\Gamma_1} \mathbf{n}_1 \cdot h_g(T_1 - T_2)\mathbf{n}_1 &= \int_{\Gamma_2} \mathbf{n}_2 \cdot h_g(T_2 - T_1)\mathbf{n}_1 \\ \int_{\Gamma_1} h_g(T_1 - T_2) &= \int_{\Gamma_2} h_g(T_2 - T_1) \end{aligned} \tag{3}$$

where the subscripts 1 and 2 represent the fuel and cladding surfaces, $\mathbf{n}$ is the normal vector, h_g is the gap conductance, and T is temperature. The above equations specify the thermal contact constraint: the heat leaving the fuel surface must equal the heat entering the cladding surface.

Taking the simplest case, let h_g represent only the gas conductance across the gap. This may be modeled using the form proposed by Ross and Stoute [2]:

$$h_g = \frac{k_g(T_g)}{d_g + C_r(r_1 + r_2) + g_1 + g_2} \tag{4}$$

where k_g is the conductivity of the gas in the gap, d_g is the gap width (computed in the mechanics solution), C_r is a roughness coefficient with r_1 and r_2 the roughnesses of the two surfaces, and g_1 and g_2 are jump distances at the two surfaces. The conductivity of the gas mixture (k_g) is computed using the mixture rule from MATPRO [3], which permits mixtures of seven gases (helium, argon, krypton, xenon, hydrogen, nitrogen, and water vapor).

Momentum conservation is prescribed assuming static equilibrium at each time increment using Cauchy's equation,

$$\nabla \cdot \boldsymbol{\sigma} + \rho\mathbf{f} = 0, \tag{5}$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor and $\mathbf{f}$ is the body force per unit mass (e.g. gravity). The displacement vector $\mathbf{u}$, which is the primary solution variable, is connected to the stress field via the strain, through kinematic and constitutive relations.

Mechanical contact between fuel pellets and the inside surface of the cladding is based on three requirements:

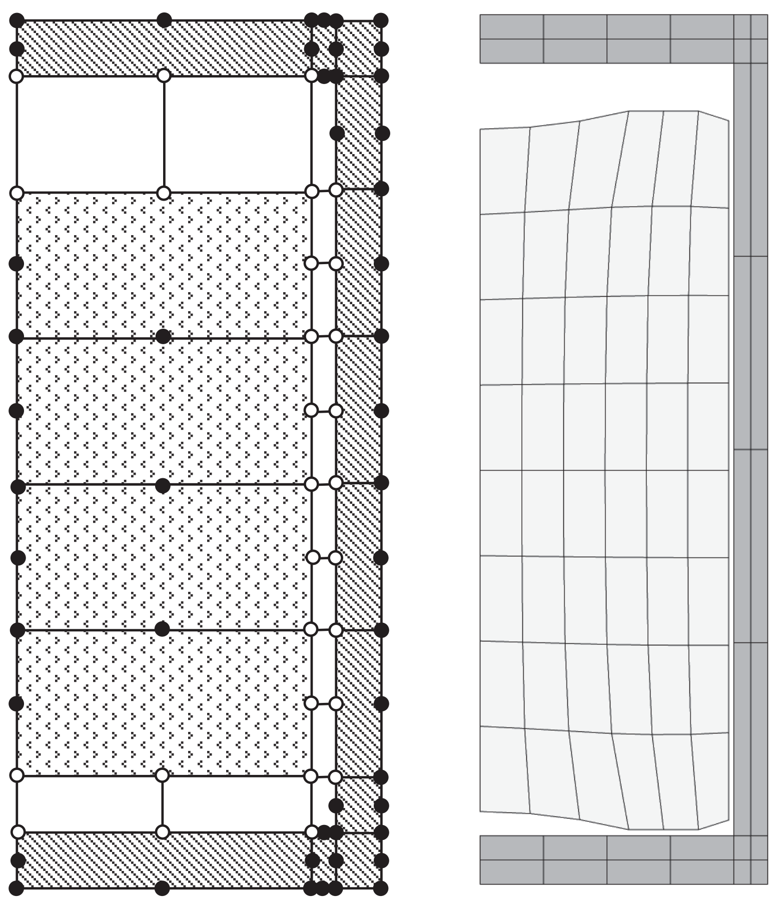
$$g \leq 0, \tag{6}$$
$$t_N \geq 0, \tag{7}$$
$$t_N g = 0. \tag{8}$$

That is, the penetration distance (typically referred to as the gap g in the contact literature) of one body into another must not be positive; the contact force t_N opposing penetration must be positive in the normal direction; and either the penetration distance or the contact force must be zero at all times.

1.2. Common Approaches to These Constraints

It is common to model the fuel-cladding system as a 1-1/2 dimensional or 2 dimensional problem. In the former approach, an axial slice of fuel is paired with an axial slice of cladding. Heat transfer from the fuel to the cladding is accomplished by introducing a one-dimensional gap heat transfer element that incorporates the gap heat conductance h_g. The result is a complete one-dimensional description of heat transfer through the fuel, gap, and cladding.

The second approach is to take an axisymmetric description of the fuel-cladding system. The fuel is typically considered to be a smeared column of fuel rather than individual fuel pellets. The fuel and cladding may be allowed to displace relative to one another. However, it is common to pair fuel nodes with cladding nodes for the purposes of heat transfer at the beginning of the analysis. Like in the one-dimensional approach, one-dimensional gap heat transfer elements may be placed between the fuel and cladding nodes. Fig. 1(a) illustrates this type of model.



(a) (b)

Figure 1. In (a), an axisymmetric model of fuel and cladding with 8-node finite elements. One-dimensional gap heat transfer elements connect fuel nodes with cladding nodes. Those nodes connected to one-dimensional elements are represented as open circles. In (b), a finite element model for which one-dimensional node-to-node gap elements are not applicable.

These modeling techniques are either difficult or not applicable for the case of complicated fuel geometries. It is not possible in general to associate a single fuel node with a single cladding node. See Fig. 1(b) for an example.

The situation for modeling mechanical contact constraints is similar. For one-dimensional slices or simple two-dimensional geometries, it is possible to introduce one-dimensional gap contact elements. However, this is not possible for more complicated geometries. In addition, simplified one-dimensional gap element approaches tie heat and force transfer between predetermined locations for the duration of the analysis, which may not be accurate for problems with significant relative motion between the fuel and cladding.

1.3. Node-face, Quadrature, and Mortar Algorithms

In order to transfer heat and force across a gap in the case of a more complex finite element mesh, we turn to a different set of techniques. In the node-face approach, the one-dimensional gap elements described above are essentially replicated between a node on one side of the gap (the fuel side in this case) and a face on the other side (the cladding side). The location at which the heat or force is transmitted on the face must be determined by a search algorithm, and that location is allowed to change as the analysis progresses.

For the transfer of heat across a gap, it is convenient to model Eq. 3 by combining the search ideas of the node-face approach with integration on the two gap boundaries. This integration happens, of course, at quadrature points, and the resulting technique is referred to here as a quadrature approach.

It is also possible to formulate these constraints according to the so-called mortar method. This case can be viewed as a generalization of the quadrature approach and is applicable to both heat and force transfer.

These techniques are explained in more detail in the following section. Section 3 demonstrates the applicability of these approaches to fuel performance modeling.

2. CONTACT ALGORITHMS

This section reviews approaches that are applicable for heat and force transfer across a gap given a general finite element mesh.

2.1. Node on Face

In the node-on-face technique nodes on one side of the interface are constrained in some way to a face on the other side of the interface (see, for example, [4]). Search algorithms are required to determine the pairing of nodes to faces. The output of these algorithms are data such as the pairings themselves, the distance between the node and the face, the parametric coordinates of the point on the face closest to the node, and the normal at those parametric coordinates.

The penalty formulation is perhaps the most straightforward way to enforce node-on-face constraints. Taking mechanical contact as an example, we form the normal contact force as

$$t_N = \epsilon g. \tag{9}$$

That is, the contact force is a penalty parameter ϵ times the penetration of the node into the face. Upon inspection it will be seen that this formulation requires penetration in order to generate force opposing the penetration. With a sufficiently high penalty parameter, converged solutions will have negligibly small penetration. However, care must be taken not to choose such a high value for the penalty parameter that the solve of the system of linear equations suffers.

2.2. Quadrature

The quadrature approach to thermal contact is based on Eq. 3. The equation is evaluated at integration locations. This requires that the gap conductance h_g and the temperature across the gap be known at those integration locations. This implies that the search capability must be able to return not only node-on-face interaction data but quadrature point-on-face interaction data as well.

As will be shown, the quadrature approach gives good results on higher-order meshes, which is not the case for the node-on-face approach.

2.3. Mortar

The mortar method[5], [6] is a special technique to enforce constraints in the discretized system for non-matching meshes. The method is often implemented with Lagrange multipliers such that special interpolation functions are used to dicretize the Lagrange multiplier in the interface. The interface must be defined in a way that one side is marked as *mortar* (or *master*) and the other as *non-mortar* (or *slave*).

The basic formulation, starting from the Langrange multiplier method, adds an extra term into the weak formulation

$$\Pi_C = \int_{\Gamma_C} \lambda \, g \, dA \tag{10}$$

where C represents the master/slave interface.

The variation of Π_C leads to

$$C_C = \int_{\Gamma_C} \lambda \, \delta g \, dA + \int_{\Gamma_C} \delta\lambda \, g \, dA \tag{11}$$

where the the first term is associated with work of the Lagrange multipliers and the second enforces the constraints.

3. NUMERICAL EXAMPLES

This section demonstrates the effectiveness of the advanced contact techniques for a variety of problems.

3.1. Mechanical Contact

Figure 2 illustrates differences between a discrete and smeared-pellet analysis. The inset shows radial displacement contours and the displaced shape of a pellet at the end of power-up. Displacements are magnified 100x to show the pellet “hourglass” shape which results from thermal expansion. Due to this shape, the ends of the pellet contact the clad earlier than the pellet middle, with contact separated by about

2.5 MWd/kgU. As expected, contact in the smeared-pellet calculation falls midway between the end and middle discrete-pellet locations.

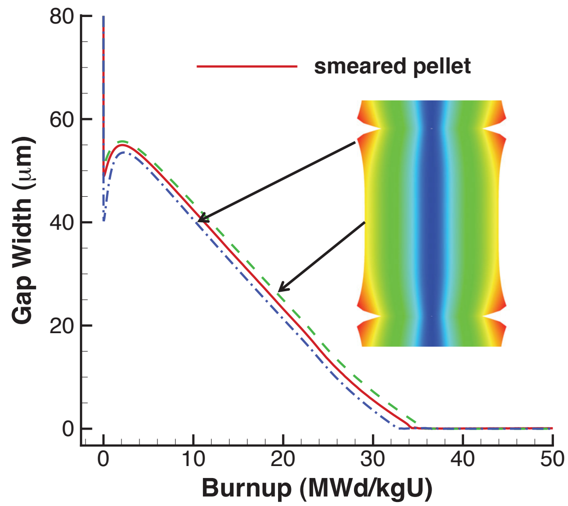


Figure 2. Rodlet results showing history of gap closure at the end and middle of a discrete pellet. Results from both the discrete and smeared-pellet calculations are shown for comparison. Inset is colored by radial displacement.

Figure 3 is a plot of the clad radial displacement versus axial length, at various times in fuel life. Results from both the discrete and smeared-pellet calculations are shown for comparison. During initial power-up, the clad displaces uniformly outward due to thermal expansion and an increase in rod pressure. Then, during the first 13 MWd/kgU of burnup, clad creep-down results in an inward displacement of approximately 13 μm. It is interesting to observe that for the discrete pellet simulation, a small pellet-to-pellet displacement oscillation is evident in the cladding, well before any contact with the fuel. This displacement oscillation is the result of an axial temperature variation in the clad of the same frequency, occuring due to reduced radial heat transfer in regions adjacent to the fuel chamfering. Gap closure and mechanical contact occur at approximately 35 MWd/kgU, as was shown in Figure 2, causing the clad to reverse direction and begin displacing outward. For the discrete-pellet simulation, localized peaks form at pellet-pellet interfaces (the “triple point”) due to the hourglass shape of the pellets. The commonly observed “bamboo” profile along the clad length is obvious.

3.2. Thermal Contact

In the node-face approach to thermal contact, the heat flux across the fuel surface is transferred to the cladding at fuel node locations. This approach works well in many cases but is problematic with higher-order finite elements. As a demonstration problem, consider the finite element model in Figure 4(a). A block with a fixed temperature (roughly analogous to a fuel pellet) is placed near a cylindrical wall (analogous to the cladding wall). The node-face approach to heat transfer produces a noisy clad wall surface temperature profile.

The approach in Figure 4(b) is to integrate the heat flux on both surfaces where the gap temperature and gap distance is computed at each Gauss point on each surface. The constraint is enforced due to the effect

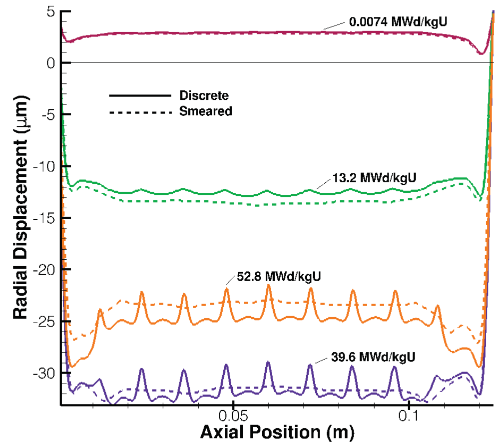


Figure 3. Clad radial displacement, versus axial length, at various times in fuel life. Results from both the discrete and smeared-pellet calculations are shown for comparison.

of the gap temperature. As can be seen by the figure, the result is a smooth temperature profile on the cladding surface.

3.3. Mortar Method

As an example of the mortar method applied to thermal contact, consider Figure 5. This problem involves a temperature gradient across a mesh composed of two domains. The interface between the domains is curved with the constraint that the temperature must match across the interface. The mortar method is able to capture the analytical solution.

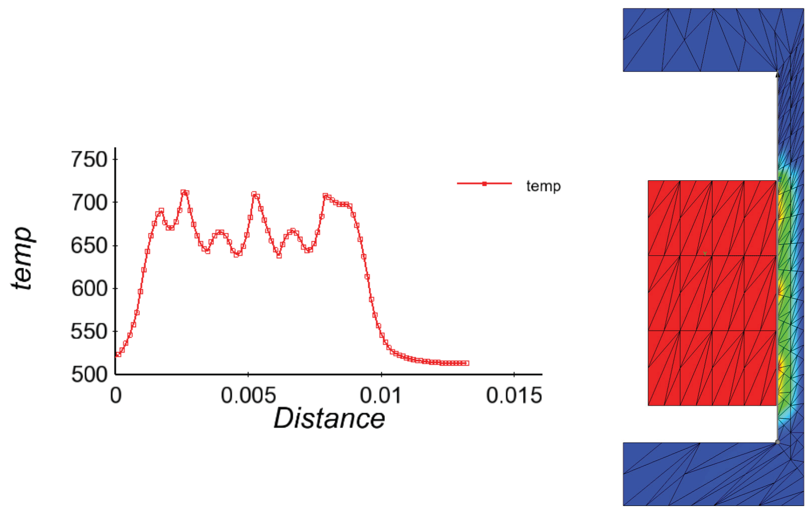
In nuclear fuel performance modeling, it is important to model gap heat transfer including a gap conductance. The mortar method is also applicable to this constraint. As a simple demonstration, consider a one-dimensional case where three zones have three conductivities (1000, 100, 500). The lengths of the zones are 0.4, 0.2, and 0.4 units. A fixed temperature is assigned to each end of the domain such that a temperature gradient develops. Using a finite element mesh in each zone, a typical solution is shown in the top portion of Figure 6(a).

With the mortar method, it is possible to remove the finite element mesh from this middle zone and enforce the thermal constraint with Lagrange multipliers. The result is shown in the bottom portion of Figure 6(a). The mortar method result matches the previous result obtained with a mesh throughout the domain, as demonstrated Figure 6(b).

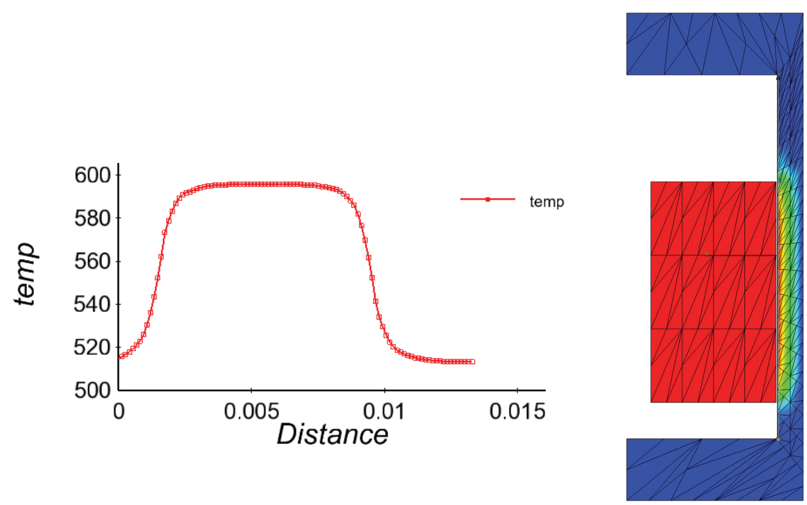
Work is underway to extend the mortar method to allow it to be used in nuclear fuel simulations.

4. CONCLUSIONS

For general meshes of fuel and cladding, it is not possible to assign node pairs for the purposes of thermal and mechanical contact. Even for simplified meshes where this is possible, the transfer of heat and force



(a) Node-face algorithm



(b) Symmetric Gauss point algorithm

Figure 4. Gap heat transfer results for two algorithms for a problem using Quad8 elements. The fuel temperature is fixed. The temp vs. Distance plots show the clad temperature upward along the inner wall. Meshes are colored by temperature. The symmetric Gauss point algorithm produces a smooth solution.

between predetermined nodes limits the accuracy of the model.

More flexible techniques provide an option for analyzing more complicated fuel geometries and to analyze them in greater detail. These techniques require a search capability to pair features on one side of the gap with features on the other. With these evolving pairings, it is possible to enforce thermal and mechanical constraints accurately and robustly.

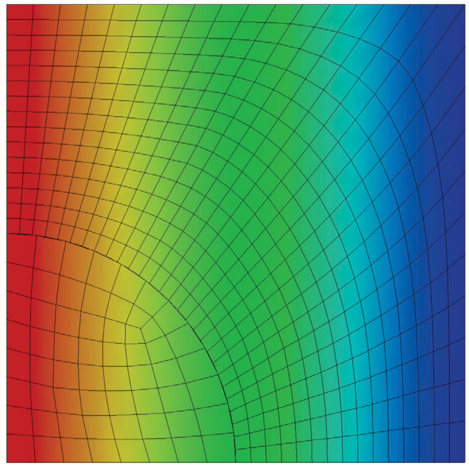
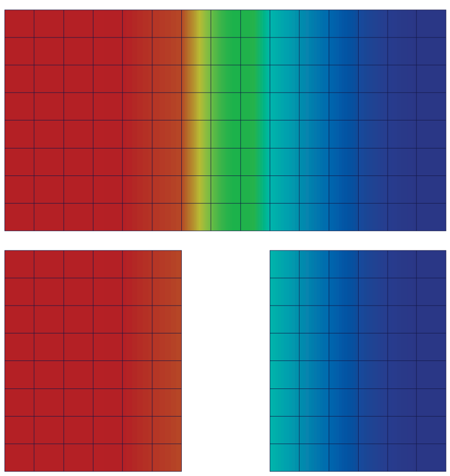
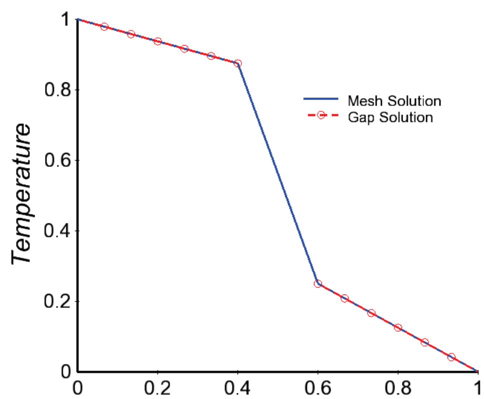


Figure 5. Linear temperature gradient across mismatched mesh boundary. The mortar method reproduces the analytical solution.



(a) Heat conduction with meshed gap (top) and mortar method (bottom).



(b) Plot of temperature vs. distance.

Figure 6. Comparison of mortar method for gap heat transfer to a meshed gap.

Node-on-face techniques are particularly helpful for mechanical constraints. A quadrature-based gap heat transfer method has been shown to be a powerful approach. Mortar methods, still in development, are proven techniques applicable to both thermal and mechanical contact. The mortar method is also a useful approach in other contexts.

ACKNOWLEDGEMENTS

The submitted manuscript has been authored by a contractor of the U.S. Government under Contract DE-AC07-05ID14517. Accordingly, the U.S. Government retains a non-exclusive, royalty free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.

REFERENCES

[1] R. Williamson, J. Hales, S. Novascone, M. Tonks, D. Gaston, C. Permann, D. Andrs, and R. Martineau, "Multidimensional multiphysics simulation of nuclear fuel behavior," *Journal of Nuclear Materials*, **423**, pp. 149–163, 2012.

[2] A. M. Ross and R. L. Stoute, "Heat transfer coefficient between UO_2 and Zircaloy-2," Tech. Rep. AECL-1552, Atomic Energy of Canada Limited, 1962.

[3] C. M. Allison and et al., "SCDAP/RELAP5/MOD3.1 code manual volume IV: MATPRO," Tech. Rep. NUREG/CR-6150, Idaho National Laboratory, 1993.

[4] M. Heinstein and T. Laursen, "An algorithm for the matrix-free solution of quasistatic frictional contact problems," *Int. J. Numer. Meth. Engrg.*, **44**, pp. 1205–1226, 1999.

[5] F. Belgacem, "The mortar finite element method with lagrange multipliers," *Numerische Mathematik*, **84**, no. 2, pp. 173–197, 1999.

[6] B. Wohlmuth, "A mortar finite element method using dual spaces for the lagrange multiplier," *SIAM Journal on Numerical Analysis*, **38**, no. 3, pp. 989–1012, 2000.