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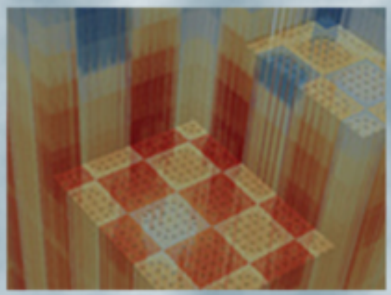
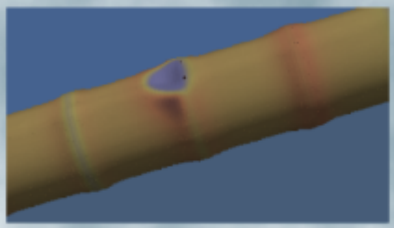
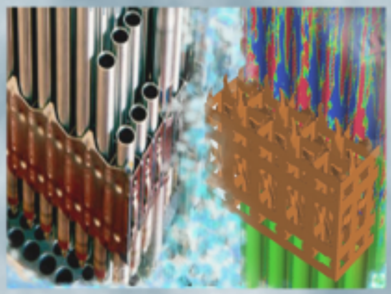
Use of Neutron Flux Calculated by Shift in a Grizzly Reactor Pressure Vessel Fracture Simulation







Benjamin W Spencer
William M Hoffman
Benjamin S Collins
Shane C Henderson

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Benjamin W Spencer, William M Hoffman
Idaho National Laboratory
P.O. Box 1625
Idaho Falls, ID 83415-3840

Benjamin S Collins, Shane C Henderson
Oak Ridge National Laboratory
1 Bethel Valley Rd,
Oak Ridge, TN 37830

September 3, 2019

1 Introduction

The reactor pressure vessel (RPV) plays the critical role of containing the reactor and coolant in a light water reactor (LWR) nuclear power plant, and must be able to safely perform this function under a variety of normal and off-normal transient loading conditions. The RPV is subjected to harsh environmental conditions (elevated temperature and high neutron flux) whenever the plant is operating, which leads to embrittlement of the steel over time. RPVs contain populations of flaws introduced during the manufacturing process, and the primary safety concern is that during a transient event, a fracture could initiate at the site of one of these flaws and lead to rupture of the RPV. RPVs are very rugged structures, and the probability of this occurring is very low. However, as the RPV's steel becomes embrittled over time, its resistance to fracture decreases and this becomes more likely. If the RPV's susceptibility to fracture increases to an unacceptable level, it will most likely lead to closure of the plant because of the extreme difficulty of repair or replacement.

Assessing the likelihood of RPV fracture during a transient event involves performing a probabilistic fracture mechanics (PFM) analysis, in which random sampling procedures are used to generate populations of pre-existing flaws, the probability of fracture of each of these flaws evaluated, and and overall probability of fracture of any flaw is computed. This is typically done using a combination of a model of the thermo-mechanical response of the RPV and reduced order models that are used to rapidly compute stress intensity factors for individual flaws. A capability to perform PFM analysis has been developed in the Grizzly code with funding from the U.S. Department of Energy's Light Water Reactor Sustainability (LWRS) program over the last several years. Grizzly offers unique capabilities for 1D, 2D, or 3D representations of the RPV and is able to take advantage of parallel computers, which are largely provided by the MOOSE framework that it is based on. Because of these capabilities, Grizzly is uniquely positioned to address aspects of this problem that can only be addressed with a higher-dimensional model.

One of the important inputs to Grizzly is the spatial distribution of the neutron fluence, which has a large impact on the material embrittlement. Prior to the work documented in this report, Grizzly obtained the fluence through a user-input value at the RPV inner surface, and used a simple attenuation law to compute the through-wall variation of the fluence. The RPV can be divided into regions where different fluences are prescribed, as is common in PFM codes. Because the fluence has such an important effect on the material embrittlement, to do an accurate analysis of the effect of the operating environment on the RPV's integrity, it is important to use a fluence distribution that is as accurate as possible.

The VERA core simulator developed by the CASL program takes advantage of high performance computing resources to perform high-fidelity multiphysics simulations of reactor physics, including the effects of neutron transport, fuel performance, and thermal hydraulics. Recently a capability was developed to also evaluate neutron fluxes away from the reactor core through the Shift code. This allows for a detailed 3D map of the spatial variation of the fluence in components such as the RPV to be computed, which is ideal for use with the Grizzly code.

This report documents an initial effort to couple the neutron transport calculations performed in VERA/Shift with Grizzly. This allows Grizzly to take advantage of a highly detailed fluence map in its calculation of the effect of environmental exposure on propensity for fracture.

2 Summary of Grizzly probabilistic fracture mechanics algorithms

The procedures used by Grizzly for PFM calculations are described in detail in [1]. It is important to emphasize that Grizzly largely implements the same algorithms that were originally developed in the FAVOR code [2, 3], which are the result of decades of research on fracture in heavy section steel carried out at Oak Ridge National Laboratory.

The steps of the PFM calculation can be summarized as follows:

1. **Global thermomechanical response analysis**: The parameters that affect fracture of individual flaws (stress intensity factor and temperature) are driven by the through-wall stress and temperature distributions, which are computed for each time step during a transient loading event using a global finite element model of the RPV. This can be done using a 1D, 2D, or 3D model as appropriate for the phenomena being considered. Grizzly uses the tightly-coupled multiphysics solution capabilities provided by MOOSE to perform this calculation.

2. **Probabilistic fracture mechanics analysis**: This step uses Monte Carlo sampling to generate a set of random realizations of a population of flaws. Each one of these realizations is a physically reasonable representation of the set of flaws that would be expected to be observed in the RPV. The randomized variables describing each flaw include flaw location and dimensions, local fluence and concentrations of alloying elements, and the unirradiated nil-ductility reference temperature, RT_{NDT}, which is a measure of the brittleness of the steel. Once these parameters are generated, reduced order fracture mechanics models are used to rapidly evaluate the mode-I stress intensity factor, K_I for each flaw during each time step of the transient event using information from the global RPV thermomechanical model. The embrittlement, measured in terms of the shift in RT_{NDT} is computed using a model such as that of [4, 5]. From K_I and the local temperature and RT_{NDT}, the conditional probability of fracture initiation, CPI for each flaw is computed. The aggregate CPI for the entire vessel, $\mathrm{CPI}_{\mathrm{RPV}}$ is computed from the CPI of individual flaws:

$$\mathrm{CPI}_{\mathrm{RPV}} = 1 - \prod_{i=1}^{n_{\mathrm{flaw}}} (1 - \mathrm{CPI}_i) \tag{1}$$

   where n_{flaw} is the total number of flaws in the RPV and CPI_i is CPI for each flaw with index i.

3. **Postprocessing of probabilistic analysis results**: Ultimately, the quantity of interest is the probability of failure of the RPV under the variety of transient events that could occur, each of which has its own CPI and probability of occurrence. This can be computed by taking the sum of the products of the probability of occurrence of each transient and its associated CPI. Also, to understand better the types and locations of dominant flaws, it is helpful to visualize the properties of the individual flaws with nonzero CPI.

Grizzly uses a modular system for the various components of the PFM calculation. This makes it straightforward to use different models or methods of computation for the various elements of the calculation. This property of Grizzly makes it straightforward to modify it to obtain the fluence from Shift.

3 VERAShift overview

An emerging capability in VERA development is the ability to compute vessel fluence [6]. This capability leverages the core simulation capability of VERA through MPACT, CTF, and ORIGEN; and sends the neutron source to Shift which will transport the neutrons to the vessel and into the regions outside the core. Shift leverages the CADIS (Consistent

Adjoint-Driven Importance Sampling) methodology to decrease the uncertainty of the flux in the vessel caused by the stochastic variance of the calculation.

The VERAShift calculation sequence begins with the standard MPACT/CTF solve for a single statepoint. MPACT and CTF iterate until the power, density, and temperature fields in the core have converged. Before MPACT performs a timestep, the pin-by-pin isotopic fission rates are passed to Shift. Shift uses the isotopic fission rates to sample from the Watt spectrum specific to that isotope to determine the neutron source. Shift then uses the variance reduction parameters computed by CADIS to transport the neutrons through the geometry and compute radial, azimuthal, and axial flux in the vessel region. While the Shift calculation is running, MPACT advances its timestep using ORIGEN and solves the next statepoint with another coupled MPACT/CTF run. MPACT then waits for the Shift calculation to finish, receives the flux and variance distribution in the vessel from Shift, and time integrates over the timestep. This sequence is continued for the entire cycle. MPACT also stores the vessel fluence and variance information on its restart file so the vessel fluence can be easily accumulated over multiple cycles of operation.

4 Process to transfer fluence from VERAShift to Grizzly

The fluence is transferred between the codes in this work via an Exodus II file [7], which is a database format designed to store mesh topology and field data for input and output of finite element analysis codes and other codes that use unstructured meshes. A mesh is constructed to cover the volume of the region of the RPV to be considered. A field variable that stores the value of the fluence at every node in that mesh is included with the mesh. The standard finite element interpolation functions can be used within Grizzly to evaluate the value of the fluence at any point in the region of interest of the RPV for use in the embrittlement calculation.

Exodus II is one of the file formats that is well-supported for input and output in Grizzly and other MOOSE-based codes. VERA does not natively output results in Exodus II format, so a standalone program was written to convert fluences from VERA's native HDF5 output format to Exodus II. This program was written in Python, and makes use of `exodus.py` [8], which provides Python bindings for the application programming interface (API) to the Exodus II library. This Python program loops through the nodes of the Exodus mesh, calls functions to evaluate the values of the fluence field, and saves those to the Exodus mesh file.

Figure 1 shows the modular structure of the components used by Grizzly for PFM calculations. Each of the boxes in this diagram represents a C++ base class from which specialized classes are derived to provide this functionality in various ways. Prior to this work, there was only one class derived from FluenceCalculator to compute the fluence at the locations at specific flaws. This class, called FluenceAttenuatedFromSurface, uses a user-supplied uniform fluence specified over a region of the RPV, and attenuated that fluence through a simple exponential law through the wall thickness. For the present work, a new class called FluenceFromFieldValue, shown in the diagram on the right in Figure 1, which obtains the fluence from a FieldValueCalculator class. FieldValueCalculator is a base class from which multiple classes are derived that allow for a field value to be defined in various ways, including using a value interpolated from a field read from an Exodus II file.

5 Demonstration applications

The Shift/Grizzly coupling capabilities are demonstrated here on a model of the beltline region of a representative pressurized water (PWR) reactor RPV. The region of the RPV in the vicinity of the core experiences the highest fast neutron fluence, and typically only that region is considered in an RPV PFM analysis. The configuration of the plates or forgings the comprise the RPV, as well as the welds between these regions, has a significant effect on the integrity of the RPV. A single fluence map obtained from Shift is used in a PFM analysis of three different RPVs with various configurations of these regions.

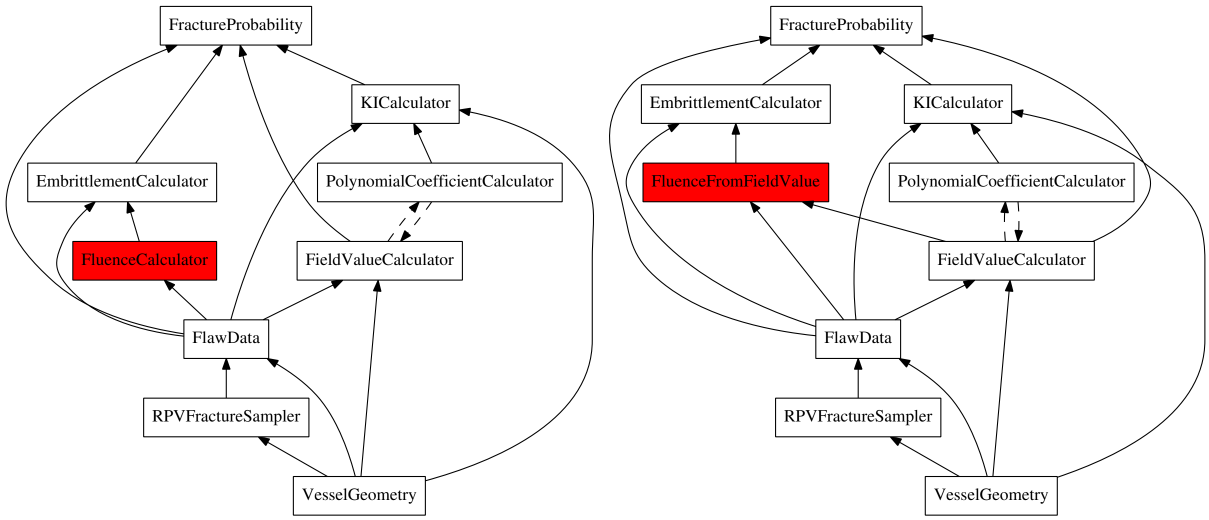

Figure 1: Modular structure of the components of the Grizzly PFM capability, showing the dependencies between these components (adapted from [1]). (left) Diagram of the dependencies between the basic types of these components, with the FluenceCalculator component highlighted. (right) The same dependency diagram showing the use of the FluenceFromFieldValue specialized class developed for this application. Note the dependency of FluenceFromFieldValue on FieldValueCalculator, which provides much of the required functionality.

5.1 Fluence map

Figure 2 shows the fluence map from Shift mapped onto the Exodus II file used by Grizzly to define the spatial fluence variation. The image on the left of Figure 2 shows the fluence as calculated by Shift after 411 effective full power days. For this study, it is assumed that the vessel is subjected to 40 effective full power years to illustrate the effect of the fluence on RPV integrity after a significant operational life. The Shift-calculated is extrapolated to 40 effective full power years as shown in the image on the right of Figure 2 by simply multiplying it by a constant factor to account for the longer operation time, and this fluence is used in these calculations.

5.2 RPV structural models

RPVs are constructed of either plates or forgings welded together, and Grizzly has models for the embrittlement of welds, plates, and forgings. Three different RPV region layouts are considered here to illustrate the relative behavior of these types of materials. The first RPV considered is shown in Figure 3 and is composed of a single plate region. This is not a realistic configuration, as multiple plates must be welded together to form an RPV, but is useful for demonstration purposes. The second RPV configuration, shown in Figure 4 consists of two forgings separated by a single circumferential weld. The third RPV model is made up of six plates joined together by six axial welds (three on the bottom half and three on the top half, offset by 60 degrees) and one circumferential weld, shown in Figure 5.

The same RPV dimensions were used for all three models. The inner radius of the vessel is 2.1915 meters, the cladding thickness is 0.0056 meters and the total wall thickness is is 0.225 meters. The height of the region considered for the RPV integrity analysis is 4.13937 meters. and is not meant to represent the entire beltline region of an RPV, rather the area most affected by the neutron flux. The RPV is assumed to be subjected to uniform thermal and pressure loading over the entire beltline region, so a 1D Grizzly model was used to represent the global thermomechanical response of the RPV.

It is important to note that the intent of this study is primarily to demonstrate the coupling between Shift and Grizzly, and not to evaluate an actual RPV. In selecting model dimensions and material properties, properties consistent with those of actual operating PWRs, which are documented in the Reactor Vessel Integrity Database [9] were used but are not for a specific plant. To fully characterize the regions that make up the RPV, it is necessary to define mean values

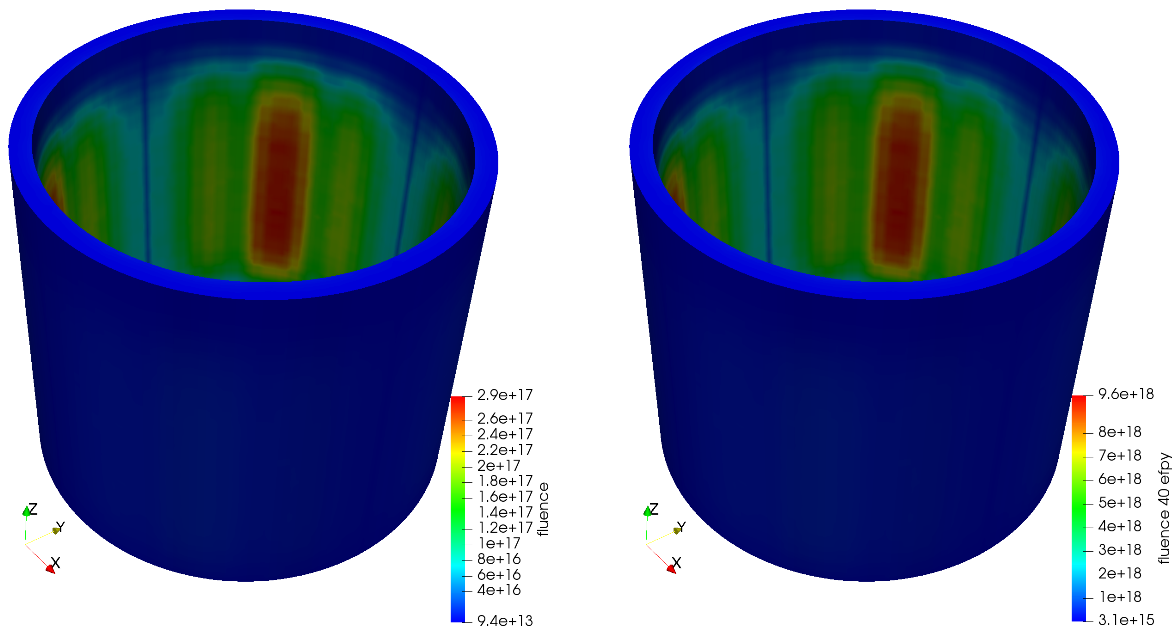

Figure 2: Fluence map provided by Shift to Grizzly, shown in units of neutrons/cm^2 of neutrons > 1MeV. (left) Fluence after 411 effective full power days. (right) Fluence extrapolated to 40 effective full power years.

Figure 3: Schematic of rollout of RPV beltline region with entire RPV represented as a single plate

Figure 4: Schematic of rollout of RPV beltline region containing two forgings and a circumferential weld

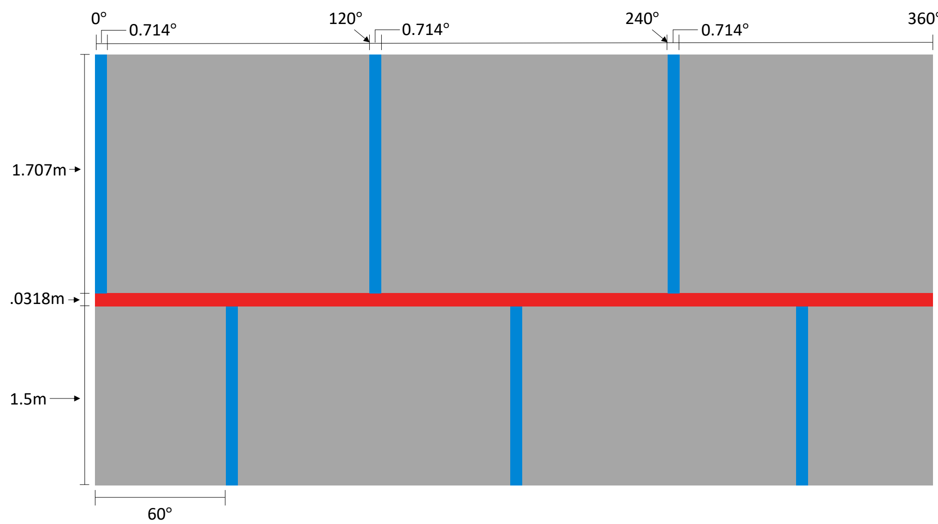

Figure 5: Schematic of rollout of RPV beltline region containing multiple plates and axial and circumferential welds

of concentrations of alloying elements and the initial value of RT_{NDT}. Table 1 shows the values of these parameters used in all of these models for the various region types.

Table 1: Mean values of key material properties used for the region types in demonstration RPV simulations

Material	**Cu (wt%)**	**Ni (wt%)**	**Mn (wt%)**	**P (wt%)**	**Initial RT_{NDT} (°F)**
Plate	0.13	0.7	1.44	0.01	50
Forging	0.13	0.7	1.44	0.01	50
Weld	0.13	0.1	1.44	0.01	-50

RPV fracture is often dominated by the behavior of the weld regions because they tend to be more susceptible to embrittlement, and it will be seen that this is the case in the present analyses. This is despite the fact that as seen in Table 1, the initial RT_{NDT} is significantly lower for the welds than for the plates and forgings (lower values of RT_{NDT} indicate greater toughness), which is often the case in actual RPVs.

Figure 6: Convergence history of Monte Carlo iterations for computation of the mean CPI for the the three RPV configurations considered here

All RPVS use the same representative data describing the distribution of flaws through the vessel in the weld and plate/-forging regions. For simplicity, this study only considered embedded flaws, although Grizzly does have a capability to consider distributions of surface-breaking flaws as well. The RPVs are all subjected to the same transient loading event, which is a particularly aggressive transient taken from a loading scenario considered in an actual plant, and uses the same temperature and pressure history used in the demonstrations of Grizzly in [1].

5.3 Results

For each of the three RPV configurations, a PFM analysis was performed using 100000 RPV realizations in the Monte Carlo analysis. Figure 6 shows the running history of the mean CPI for each of these cases, and illustrates how a large number of RPV realizations is required to achieve convergence. Many realizations have no flaws with a nonzero CPI, so there is significant noise early on in this iteration history. As expected, the cases with multiple plates or forgings and welds have significantly higher CPI than the case with only the plate region because the weld regions dominate the calculations. The forgings had lower embrittlement than the plates in this case, and there were fewer welds in the forging case than in the case with multiple plates, which led to a lower CPI for the forging case. In interpreting these results, it is important to recognize that this is a particularly aggressive transient with a low likelihood of occurrence, so these results by themselves do not indicate that the RPV has a high likelihood of fracture during operation.

Visualizing the locations of the flaws with high CPI is very helpful for understanding the effects of the local environment on fracture. Figures 7, 8, and 9 show the population of flaws with nonzero CPI for 100000 RPV realizations for each of the three RPV configurations considered, visualized in three different ways. In one set of plots, the flaws are shown in 3D coordinates superimposed on a partially translucent image of the RPV with the fluence map. Two 2D plots are also shown for each case, one showing the flaws plotted in terms of depth from the inner wetted surface of the RPV and azimuthal position, and the other showing the flaws plotted in terms of axial position and azimuthal position. In both of these sets of 2D plots, the flaws are colored according to their CPI. These sets of plots are very helpful in understanding how the flaws with high probability of failure are clustered, which occurs at areas with high embrittlement.

Figures 7, 8, and 9 show some notable trends. The plate-only case in Figure 7 clearly shows how the flaws with higher failure probability are clustered in the regions where the fluence is high. The flaws near the inner surface of the vessel tend to be more likely to fail both because the embrittlement is higher and because they are subjected to more aggressive loading conditions than deeper flaws during the transient event. When welds are included, as in Figures 8 and 9, the clustering of flaws with high CPI is clearly focused in the weld regions, and the weld regions that coincide with high neutron have especially high concentrations of flaws with high CPI.

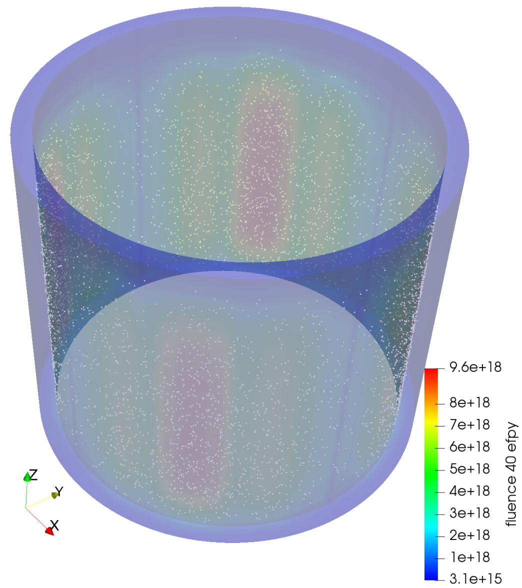

Figure 7: Scatter plots of the population of flaws with nonzero CPI from 100000 random realizations of the flaw population for the RPV represented as a single plate (Figure 3). (top) Flaw locations shown as white dots superimposed on the 3D fluence map, (middle) Flaws colored by CPI plotted in terms of through-wall depth vs. azimuthal position, (bottom) Flaws colored by CPI shown plotted in terms of axial position vs. azimuthal position.

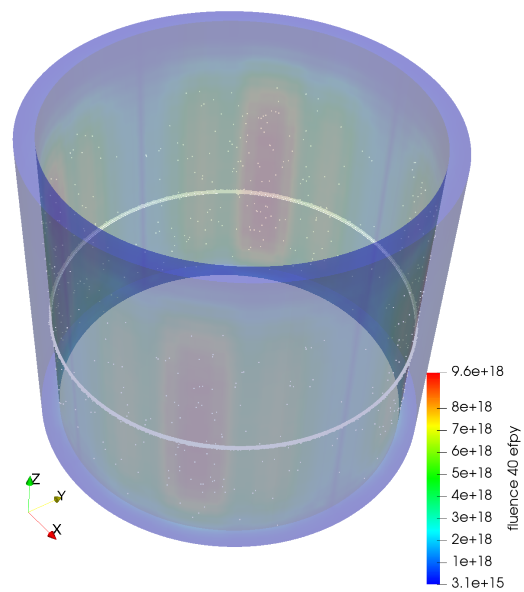

Figure 8: Scatter plots of the population of flaws with nonzero CPI from 100000 random realizations of the flaw population for an RPV comprised of two forgings and a circumferential weld (Figure 4). (top) Flaw locations shown as white dots superimposed on the 3D fluence map, (middle) Flaws colored by CPI plotted in terms of through-wall depth vs. azimuthal position, (bottom) Flaws colored by CPI shown plotted in terms of axial position vs. azimuthal position.

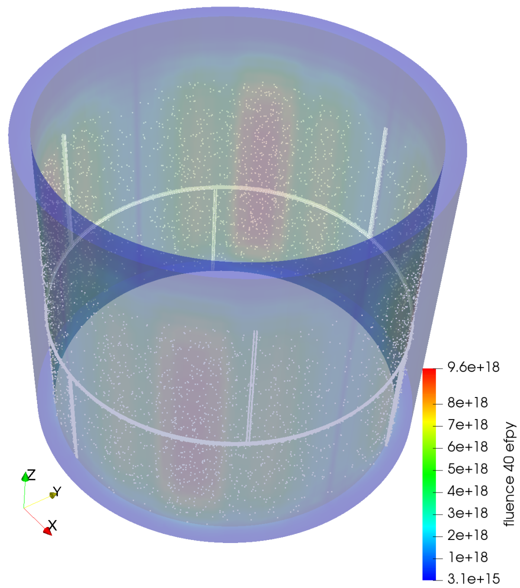

Figure 9: Scatter plots of the population of flaws with nonzero CPI from 100000 random realizations of the flaw population for an RPV comprised of multiple plates and axial and circumferential welds (Figure 5). (top) Flaw locations shown as white dots superimposed on the 3D fluence map, (middle) Flaws colored by CPI plotted in terms of through-wall depth vs. azimuthal position, (bottom) Flaws colored by CPI shown plotted in terms of axial position vs. azimuthal position.

6 Summary and future work

This report documents the procedure developed to perform a first of its kind simulation that couples an ex-core fluence calculation performed based on a high fidelity multiphysics core physics simulation and a probabilistic fracture mechanics simulation of the embrittled RPV. This was done by developing a tool to map results from the Shift code to and Exodus II mesh file, and by adding a capability in Grizzly to read the fluence from this file.

The proof-of-concept simulations shown here clearly demonstrate the importance of including a realistic representation of the spatial variation of the fluence in a probabilistic fracture mechanics simulation. The regions with both high fluence and materials that are more susceptible to embrittlement clearly have the highest concentrations of flaws with an increased potential for fracture. Including this kind of fidelity in a fluence map used in a fracture mechanics calculation can clearly lead to more accurate results when considering RPV integrity for long term operation of existing nuclear power plants.

This work demonstrates the power and flexibility of Grizzly's architecture for PFM simulations. There are multiple areas for potential future research to build on this work:

- The simulations here assume uniform thermal conditions on the inner surface of the RPV, but in reality, the temperature on the inner surface can be lower near the inlets, which would lead to increased thermal stresses and lower temperatures in those areas during a transient event, both of which can increase the susceptibility of the RPV to fracture. Grizzly has a unique capability for fully 3-dimensional PFM simulations, and if provided with realistic thermal conditions, could readily be used to investigate the importance of this effect.
- The effect of irradiation on steel embrittlement is characterized only by the fast neutron fluence, which represents only part of the neutron spectrum. The Shift model provides the full neutron spectrum, and if embrittlement models were based on other measures of irradiation damage such as dpi, the effects of lower energy neutrons could be considered. This could be used to better understand the significance of fracture in regions of the RPV farther away from the core that experience higher fluxes of neutrons with lower energy relative to the fast neutron flux.
- The simulations performed here use representative parameters for a proof of concept. Including more realism in these simulations would give a better indication of the parameters that are the most important in actual operating plants, and would allow focusing future material degradation research in those areas.

7 Acknowledgments

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