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Interfacing VPSC with finite element codes: Demonstration of irradiation growth simulation in a cladding tube

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1. Introduction

Dimensional changes in Zr alloys, associated with coupled irradiation growth and creep, are detrimental to their use in cladding tubes in reactor pressure vessels [1–4]. Irradiation growth refers to the volume conserving, anisotropic shape change observed in hexagonal crystals, even in the absence of external stress [5]. Specifically, positive ‘growth’ strains observed along the a –axis of hcp crystals are attributed to the growth of interstitial loops on prism planes, while negative strains along the c –axis are attributed to excess vacancy flux to c -type dislocations and the nucleation and growth of vacancy loops on basal planes [6]. Moreover, accelerated growth rates are observed during the later stages of irradiation (generally referred to as the break-away stage of irradiation growth) and have been correlated with the appearance of vacancy loops on basal planes [7–9].

Golubov and co-authors [10–12] proposed a reaction-diffusion model that accounts for microstructure evolution with dose, and was used to predict the irradiation growth behavior of single crystal Zr. This mean field rate theory model describes the constitutive behavior of a single crystal, and does not account for texture and internal stress effects on irradiation creep and growth behavior of polycrystalline Zr alloys. In order to account for these effects, we have implemented the reaction-diffusion model in a viscoplastic self-consistent (VPSC) crystal plasticity framework [13] to predict irradiation growth in hcp polycrystals, to study the effects of various microstructural variables influencing irradiation growth and creep [14]. Specifically, texture effects, grain interactions, microstructure evolution in individual grains, and fully anisotropic response of grains and aggregate are accounted for explicitly by this approach.

The goal of the work described above is to provide CASL with constitutive laws based on physical mechanisms for describing irradiation response of Zr alloys. The ultimate goal is to interface such VPSC-based laws with FE codes capable of simulating entire fuel channels. In the current report we describe our progress along such line. Specifically, we describe how VPSC was interfaced with FE codes ABAQUS [15] and MOOSE [16], and we present benchmarks and medium complexity applications to predictions of irradiation growth and creep in a cladding tube. Though we include a brief description of single and polycrystal formulations in Section 2 and 3, the emphasis of this report is on the FE applications (Sections 4 and 5).

2. Crystallographic Model for Irradiation Growth and Creep

The reaction-diffusion model is thoroughly discussed in Refs. [10–12] and only the main characteristics and assumptions are described in what follows. The neutron flux induces radiation cascades which create vacancies, self-interstitials, and interstitial clusters. The model uses four crystallographic directions to describe strains and dislocation Burgers vectors: the three basal compact directions and the c-axis direction ($j \equiv \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{c}$). The average concentrations of vacancies and interstitials in the effective medium are denoted by c_v and c_i , respectively, and they are assumed to diffuse isotropically. The model assumes that equal number of SIA clusters are generated along each basal direction, $j \equiv \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ and keeps track of their individual concentrations, c_{ic}^j , separately. In addition, the SIA clusters diffuse uni-directionally along the basal directions $j \equiv \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$. Dislocation lines are projected along $j \equiv \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{c}$ and dislocation loops form on prism and basal planes with Burgers vectors, $\mathbf{j} \equiv \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ and $\mathbf{c}$, respectively. Absorption of point defects and SIA clusters at dislocation sinks (of density, ρ^j) leads to the climb of line dislocations and both, interstitial-type and vacancy-type loops. Interstitial clusters have a Burgers vector in the basal plane and interact only with dislocations with Burgers vector $\mathbf{b} = \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$.

Interstitial loops (with number density, N_i^j , and mean radius, r_i^j) and vacancy loops (with number density N_v^j and mean radius r_v^j) nucleate and grow in prism and basal planes, although the characteristics of the model favor net interstitial capture at loops on the prism planes, and net vacancy capture at loops on the basal planes after a certain incubation dose. The resulting climb of these sessile dislocation loops contributes to positive growth strains, $\varepsilon_g^{a_1}, \varepsilon_g^{a_2}, \varepsilon_g^{a_3}$, along the prismatic directions and negative growth strain, ε_g^c , along the basal direction. Further, the radiation induced-defects are also absorbed at grain boundaries (which have a sink strength, k_{GB}^2) [17,18], although here we do not account for the contribution to strain from this mechanism.

Summarizing, the growth rate associated with the prismatic and basal directions are given by [10,14]:

$$\dot{\varepsilon}_g^j = G_{NRT} \chi \left(\frac{1}{3} - \frac{\rho^j}{\sum_j \rho^j + k_{GB}^2} \right) ; \quad j \equiv \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3 \quad (1)$$

$$\dot{\varepsilon}_g^j = -G_{NRT} \chi \frac{\rho^j}{\sum_j \rho^j + k_{GB}^2} ; \quad j \equiv \mathbf{c} \quad (2)$$

where, $\rho^j = \rho_d^j + 2\pi r_i^j N_i^j + 2\pi r_v^j N_v^j$, ρ_d^j is the line density of dislocations present before irradiation (such as the ones introduced by cold-working), G_{NRT} is the NRT defect production rate, $\chi = (1 - \beta_r) \beta_{SIA}$, β_r is the fraction of point defects that recombine in the displacement cascades, β_{SIA} is the fraction of interstitials that form SIA clusters, and k_{GB}^2 is the GB sink strength. Here the GB sink strength follows from the solution of the boundary value problem of point defects diffusing out from the center of a spherical grain of radius, R_m , with dislocation sinks in the interior and a zero concentration of point defects at the surface (cf. [18,19]). This gives a solution for the GB sink strength of the form:

$$k_{Gm}^2 = \frac{1}{R_m^2} \frac{\beta_m^2 (\beta_m \coth(\beta_m) - 1)}{\beta_m^2 - 3(\beta_m \coth(\beta_m) - 1)}; m \equiv x, y, z \quad (3a)$$

where,

$$\beta_m = \sqrt{\sum_j \rho^j R_m}; j \equiv a_1, a_2, a_3, c; m \equiv x, y, z \quad (3b)$$

Here, the GB sink strength of non-spherical grains is identified with the arithmetic mean of three GB sink strengths, each one calculated using a radius, R_m , equal to each of the three main dimensions of the grain along the m^{th} direction, as:

$$k_{GB}^2 = \frac{1}{3} (k_{Gx}^2 + k_{Gy}^2 + k_{Gz}^2) \quad (4)$$

To calculate the total growth rate, the individual contributions of each dislocation family along directions $\mathbf{b} = \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ (Eqs. (1) and (2)) have to be rotated to a common system and added up. For a reference system $\mathbf{x} \parallel \mathbf{a}_1, \mathbf{y} \parallel (\mathbf{a}_2 - \mathbf{a}_3), \mathbf{z} \parallel \mathbf{c}$ it is possible to show that the growth rates coincide with those reported by Barashev et al. (see Eqs. 16-23 in Ref. [10]), namely:

$$\begin{aligned} \dot{\epsilon}_{xx}^{(growth)} &= G_{NRT} \chi \left(\frac{1}{2} - \frac{\rho^{a_1} + \rho^{a_2}/4 + \rho^{a_3}/4}{\rho} \right) \\ \dot{\epsilon}_{yy}^{(growth)} &= G_{NRT} \chi \left(\frac{1}{2} - \frac{3\rho^{a_2}/4 + 3\rho^{a_3}/4}{\rho} \right) \\ \dot{\epsilon}_{zz}^{(growth)} &= -G_{NRT} \chi \left(\frac{\rho^c}{\rho} \right) \end{aligned} \quad (5)$$

For simplicity, the grain boundary sink strength has been assumed to be zero for deriving Eq. (5).

A single crystal subjected to applied stress will not only grow but also creep under irradiation. In a polycrystal, the incompatibility between the growth rate of the grain and the surrounding medium will induce internal stresses, even in the absence of an external stress state. These grain-level internal stresses promote irradiation creep, which tend to relax the growth-induced stresses. As a

consequence, accounting for irradiation creep is essential in any polycrystal model. We have implemented a crystallographic model for irradiation creep, inspired from the accepted empirical creep law used in steel deforming under irradiation creep and swelling (cf. [20]), but omitting the swelling term in this case. Such law assumes a linear dependence of creep rate with applied stress and radiation dose rate, $d\phi/dt$, of the form:

$$\dot{\epsilon}^{creep} = B_0 \sigma \frac{d\phi}{dt} \quad (6)$$

In our crystallographic formulation, such empirical law applies separately to each slip system. Only glissile dislocations, but not the sessile loops, are activated by the resolved shear τ^s on the slip systems, and their contribution to deformation is proportional to the relative availability of dislocations. As a consequence:

$$\dot{\gamma}^{s(creep)} = B \frac{\rho_d^s}{\sum_s \rho_d^s} \tau^s \frac{d\phi}{dt} \quad (7)$$

where, B is the crystallographic irradiation creep compliance. The dislocation dependence in Eq. (7) plays a crucial role in inducing anisotropic irradiation creep in the crystal. These constitutive models are implemented at the level of crystallographic slip systems in the grain. The VPSC framework [13] links the grain-level deformation, which is the tensorial sum of the crystallographic shearing rate over all slip systems, to the macroscopic deformation. This is done via a self-consistent calculation, wherein the deformation of each grain (a heterogeneous ellipsoidal inclusion) is solved in an effective medium that has the average properties of the polycrystalline aggregate of all grains in the medium (cf. [21,22]).

3. VPSC Framework

Here we use the anisotropic visco-plastic self-consistent (VPSC) polycrystal plasticity model developed by Lebensohn and Tomé [13] as a platform to account for texture, grain interaction with its surroundings, and for implementing the creep and growth constitutive laws discussed above for individual grains. Within VPSC, the aggregate (polycrystal) is represented by a discrete set of individual crystal orientations (grains), to which a volume fraction is assigned in order to reproduce the measured texture. The response and properties of such aggregate are given by averaging the response and the properties of the individual constituent grains. VPSC keeps track of and evolves incrementally the stress, strain, crystal orientation, activity of each slip system in each grain, dislocation density on each slip system, etc.

VPSC treats each grain as an ellipsoidal visco-plastic inclusion embedded in an effective visco-plastic medium, both having fully anisotropic properties. The effective medium represents the ‘average’ environment ‘seen’ by each grain. When stress, strain rate, or irradiation are applied to the effective medium, an interaction between medium and grain (embedded inclusion) takes place and local stresses are induced in the inclusion by the effective medium. The stresses, which follow

from solving the stress equilibrium equations, are uniform inside the inclusion, but deviate from the average stress in the medium depending on the relative properties and deformation trend of medium and inclusion. The ‘self-consistency’ of the approach consists on enforcing the condition that the average stress and strain rate over all the grains has to be equal to the boundary values imposed on the medium.

The propagation of slip dislocations induces plastic shear and no volumetric dilatation. Denoting $\mathbf{n}^s$ the normal to the slip plane, and $\mathbf{b}^s$ the direction of shear (Burgers vector), the resolved shear stress on the shear plane and along the shear direction associated with the stress tensor, σ_{ij}^c , acting on the grain is given by

$$\tau_{res}^s = b_i^s n_j^s \sigma_{ij}^c = m_{ij}^s \sigma_{ij}^c \quad (8)$$

where, the Schmid tensor $m_{ij}^s = \frac{1}{2}(b_i^s n_j^s + b_j^s n_i^s)$ projects the stress on the shear plane along the shear direction. The strain rate tensor associated with creep shear rates, $\dot{\gamma}^s$ (Eq. 7), in systems s is

$$\dot{\epsilon}_{ij}^{(creep)} = \sum_s m_{ij}^s \dot{\gamma}^{s(creep)} \quad (9)$$

Adding the growth and creep contributions (Eqs. (1), (2), and (9)), the total strain rate of the grain is

$$\dot{\epsilon}_{ij} = \dot{\epsilon}_{ij}^{(growth)} + \dot{\epsilon}_{ij}^{(creep)} \quad (10)$$

The systems that we consider in HCP Zr crystals are: glissile dislocations on $\{1010\}\langle 1120 \rangle$ prism (3 systems), $\{0001\}\langle 1120 \rangle$ on basal (3 systems), $\{1011\}\langle 1123 \rangle$ on pyramidal (12 systems). We also account for one sessile dislocation loop type $(0002)\langle 0002 \rangle$ in the basal planes, and three sessile loops $\{1120\}\langle 1120 \rangle$ in prism planes. The experimental information indicates that basal loops present a vacancy stacking fault configuration, and prism loops an interstitial stacking fault configuration.

For representing the response of the effective medium (polycrystal) we use a linear relation:

$$\bar{\dot{\epsilon}}_{ij} = \bar{M}_{ijkl} \bar{\sigma}_{kl} + \bar{\dot{\epsilon}}_{ij}^o \quad (11)$$

where $\bar{\dot{\epsilon}}_{ij}$ and $\bar{\sigma}_{kl}$ are overall (macroscopic) magnitudes and $\bar{M}_{ijkl}$ and $\bar{\dot{\epsilon}}_{ij}^o$ are the macroscopic creep compliance and macroscopic growth rate, respectively. The growth of the polycrystal takes place in the absence of applied stress but, as mentioned before, internal stresses in the grains are always present. Solving the inclusion-medium interaction leads to an ‘interaction equation’, which relates the stress and strain rate in the inclusion with equivalent average quantities in the effective medium

$$(\dot{\epsilon}_{ij} - \bar{\dot{\epsilon}}_{ij}) = -\tilde{M}_{ijkl} (\sigma_{kl} - \bar{\sigma}_{kl}) \quad (12a)$$

with
$$\tilde{M}_{ijkl} = (I - S)_{ijmn}^{-1} S_{mnpq} \bar{M}_{pqkl} \quad (12b)$$

Equation (12) indicates that the stress and the strain rate in the inclusion differ from those in the effective medium. The macroscopic moduli $\bar{M}_{ijkl}$ and $\bar{\dot{\epsilon}}_{ij}^o$ are unknown *a priori* and need to be adjusted self-consistently by enforcing the condition that the stress and strain rate averaged over all grains has to be equal to the stress and strain rate of the effective medium

$$\bar{\dot{\epsilon}}_{ij} = \langle \dot{\epsilon}_{ij}^c \rangle \quad \text{and} \quad \bar{\sigma}_{kl} = \langle \sigma_{kl}^c \rangle \quad (13)$$

The self-consistent polycrystal approach described above has been used in the past by Tomé et al. [23–25] to model irradiation creep and growth of hexagonal polycrystals. The difference with the current application is that in the aforementioned papers single crystal growth and creep were assumed to be described by constant parameters that did not evolve with irradiation. The work of Christien and Barbu [26] and Golubov et al. [12], on the other hand, account for irradiation induced evolution of microstructure but apply it to single crystal growth. The current implementation represents the first time that a polycrystal model is implemented with evolution of microstructure.

4. VPSC-Finite Element Interface

In this work, the constitutive deformation behavior of the FEs is solved at the level of grains using VPSC. Effectively, each Gauss point in the FE mesh represents a polycrystalline aggregate with associated texture. VPSC solves the local boundary conditions imposed by the interface code between VPSC and FE (referred as VPSC-FE interface from here on) and then passes the deformed (stress and strain) state of the Gauss point to the FE code, which solves for global equilibrium of deformation in the FE mesh.

VPSC has previously been interfaced with the FE code, ABAQUS [15], and implemented in the form of a User MATerial subroutine (UMAT) [27,28], and also with the BISON-CASL fuel performance code in the form of a material model [29]. In this work, a similar algorithm has been used, albeit with a modified convergence criterion.

The algorithm for the VPSC-FE interface [27] is briefly explained in the following. Before moving forward, it should be noted that standalone VPSC only solves for the viscoplastic strain corresponding to a stress state (or, vice-versa) and does not model the elastic strain. The VPSC-FE interface described here accounts for ‘macroscopic’ elastic deformation as well. Also note that VPSC solves for deformation in the local (material) coordinate system, which is then rotated to the global (component level) coordinate system for FE calculations.

An additive decomposition of the strain increment, $\Delta \boldsymbol{\epsilon}$, into the elastic, $\Delta \boldsymbol{\epsilon}^e$, and viscoplastic, $\Delta \boldsymbol{\epsilon}^{vp}$, parts is assumed in the VPSC-FE interface, i.e., $\Delta \boldsymbol{\epsilon} = \Delta \boldsymbol{\epsilon}^e + \Delta \boldsymbol{\epsilon}^{vp}$. The stress increment, $\Delta \boldsymbol{\sigma}$, corresponding to this strain increment may be used to estimate the elastic strain increment, i.e., $\Delta \boldsymbol{\epsilon}^e = \mathbf{C}^{-1} : \Delta \boldsymbol{\sigma}$, where $\mathbf{C}$ is the self-consistent elastic stiffness of the polycrystalline aggregate calculated by the VPSC code at the beginning of each deformation increment. The

history-dependent viscoplastic strain increment, $\Delta \boldsymbol{\varepsilon}^{vp}$, on the other hand, is a function of the stress state, $\boldsymbol{\sigma}$ (rather than the stress increment), and the internal state variables (ISVs) in the constitutive model.

The FE code calls the VPSC-FE interface with an estimate of the stretch increment, $\Delta \boldsymbol{\varepsilon}_{FE}$, the rigid spin increment, $\Delta \mathbf{R}_{FE}$, and the time step increment, Δt . The VPSC-FE interface then solves for $\boldsymbol{\sigma}$ corresponding to this strain increment using an iterative Newton-Raphson scheme. The trial stress at time, $t + \Delta t$, is estimated based on the elastic strain increment from the previous time step, i.e.,

$$\boldsymbol{\sigma}_{t+\Delta t} = \boldsymbol{\sigma}_t + \Delta \boldsymbol{\sigma} = \boldsymbol{\sigma}_t + \mathbf{C} : \Delta \boldsymbol{\varepsilon}^e = \boldsymbol{\sigma}_t + \mathbf{C} : (\Delta \boldsymbol{\varepsilon} - \Delta \boldsymbol{\varepsilon}^{vp}) \quad (14)$$

where, the subscript refers to the respective time increment. VPSC is called with this stress state, $\boldsymbol{\sigma}_{t+\Delta t}$, to obtain the corresponding viscoplastic strain rate, $\dot{\boldsymbol{\varepsilon}}^{vp}$. VPSC-FE interface then calculates the residual between $\Delta \boldsymbol{\varepsilon}$ and $\Delta \boldsymbol{\varepsilon}_{FE}$ according to the following expression:

$$\mathbf{X}(\Delta \boldsymbol{\sigma}) = \Delta \boldsymbol{\varepsilon} - \Delta \boldsymbol{\varepsilon}_{FE} = \mathbf{C}^{-1} : \Delta \boldsymbol{\sigma} + \dot{\boldsymbol{\varepsilon}}^{vp} \Delta t - \Delta \boldsymbol{\varepsilon}_{FE} \quad (15)$$

If the convergence criteria (described in the following) is not satisfied in increment k , a trial stress increment for the next iteration, $k+1$, is calculated as

$$(\Delta \boldsymbol{\sigma})_{k+1} = (\Delta \boldsymbol{\sigma})_k - \mathbf{J}_{NR}^{-1}((\Delta \boldsymbol{\sigma})_k) : \mathbf{X}((\Delta \boldsymbol{\sigma})_k) \quad (16)$$

where, the Jacobian, $\mathbf{J}_{NR}$, of the Newton-Raphson iteration is given as

$$\mathbf{J}_{NR}(\Delta \boldsymbol{\sigma}) = \frac{\partial \mathbf{X}(\Delta \boldsymbol{\sigma})}{\partial (\Delta \boldsymbol{\sigma})} = \mathbf{C}^{-1} + \mathbf{M} \Delta t \quad (17)$$

where, $\mathbf{M}$ is the viscoplastic tangent moduli computed by VPSC as part of the self-consistent calculations.

A weighted convergence metric (cf. [30]) is employed here to achieve faster convergence. The scalar convergence metric is weighted according to the largest component of the strain increment, $\Delta \boldsymbol{\varepsilon}_{FE}$, such that

$$\chi = \sqrt{\sum_i \sum_j \left(\frac{|\Delta \varepsilon_{FE}^{ij}|}{\max(|\Delta \varepsilon_{FE}^{ij}|)} X^{ij} \right)^2} \quad (18)$$

where, i and j denote the respective indices of the tensor quantities.

Note that VPSC computes all quantities in the local coordinate system (the one in which the texture of the cladding is referred to), while the FE code computes all quantities in the global coordinate

system. The VPSC-FE interface, therefore, rotates all deformation quantities from the global to the local coordinate system via the rotation tensor, $\mathbf{R} = \Delta\mathbf{R}_{FE} \cdot \mathbf{R}_t$ before passing them from the FE code on to VPSC (and, vice-versa). Also note that the tangent stiffness matrix, $\mathbf{C}^t$, required by some FE codes for calculation of the deformation increment for the next time step, is simply the inverse of the Jacobian used in the Newton-Raphson calculations in Eq. (17), i.e, $\mathbf{C}^t = \mathbf{J}_{NR}^{-1}$. This is therefore passed on to the calling FE code by VPSC-FE interface. The algorithm for interfacing VPSC with the FE code is summarized in Fig. 1.

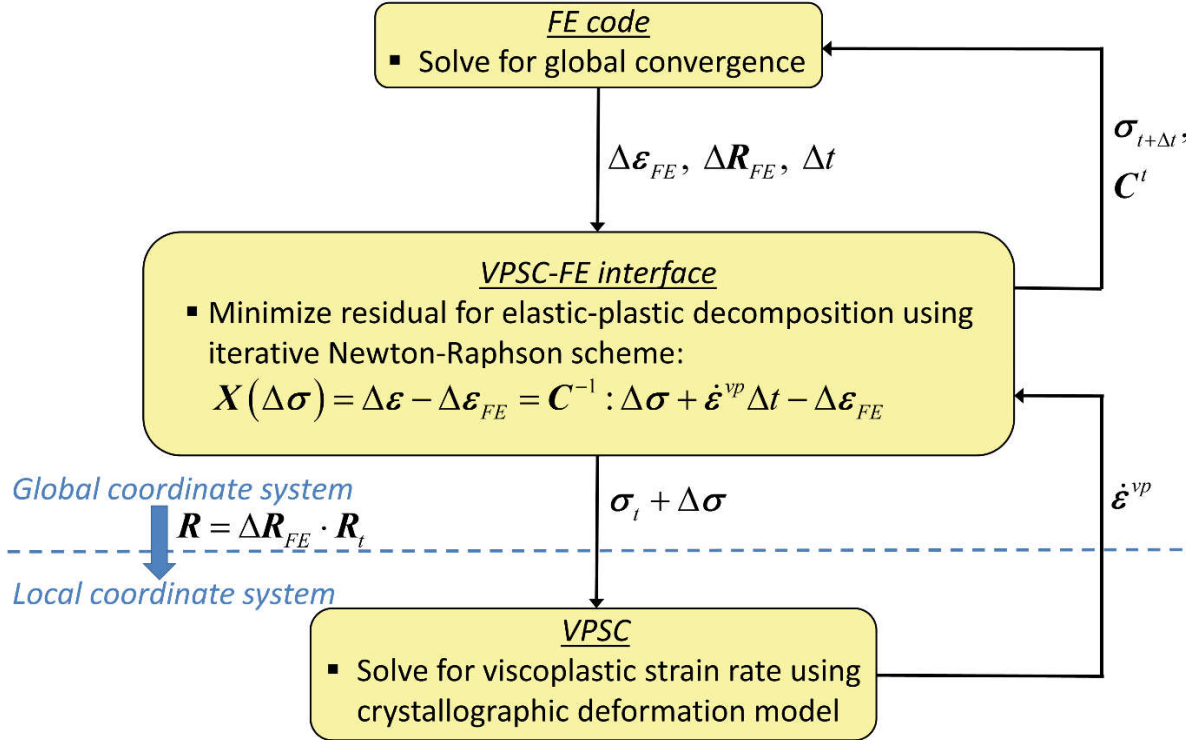


Figure 1. Algorithm for interfacing VPSC with the FE code.

5. Example Application

5.1. FE Mesh and Boundary Conditions

The VPSC-FE interface code has been implemented in a general fashion such that it can be used with ABAQUS and MOOSE FE codes (an additional wrapper code is implemented to call the VPSC-FE interface from MOOSE). This allows for benchmarking model predictions of the deformation behavior across the two different FE codes.

As an example application, irradiation growth is simulated in a cylindrical cladding tube. The tube has an outer diameter of 9.5 mm, inner diameter of 8.357 mm, and a thickness of 0.5715 mm. The length of the simulated tube is 38 mm. Given the symmetry of a cylindrical tube, a quarter geometry is used. The simulation geometry was meshed using 8-node brick elements in CUBIT

(<https://cubit.sandia.gov/index.html>) (mesh file obtained courtesy of Dr. Wenfeng Liu, Anatech Corp.) and the mesh was exported in Abaqus input (.inp) file format or in Exodus file format for use with MOOSE. Reduced integration FEs (C3D8R) were used in ABAQUS, while first order Lagrange FEs with full integration were used in MOOSE. This mesh is shown in Fig. 2 and has a total of 2400 elements, with 2 elements along the thickness. Axisymmetric boundary conditions are used such that two edges parallel to the axis of the tube are constrained in x- and y-directions, respectively. One end of the tube is constrained along the axial (z-) direction, while the other end is left free to allow for axial growth. Further, an additional node along mid-circumference is constrained at the axial end of the tube in all degrees of freedom to prevent rigid body rotation. In this example application, no external pressure was applied on the tube. These boundary conditions are highlighted in Fig. 2.

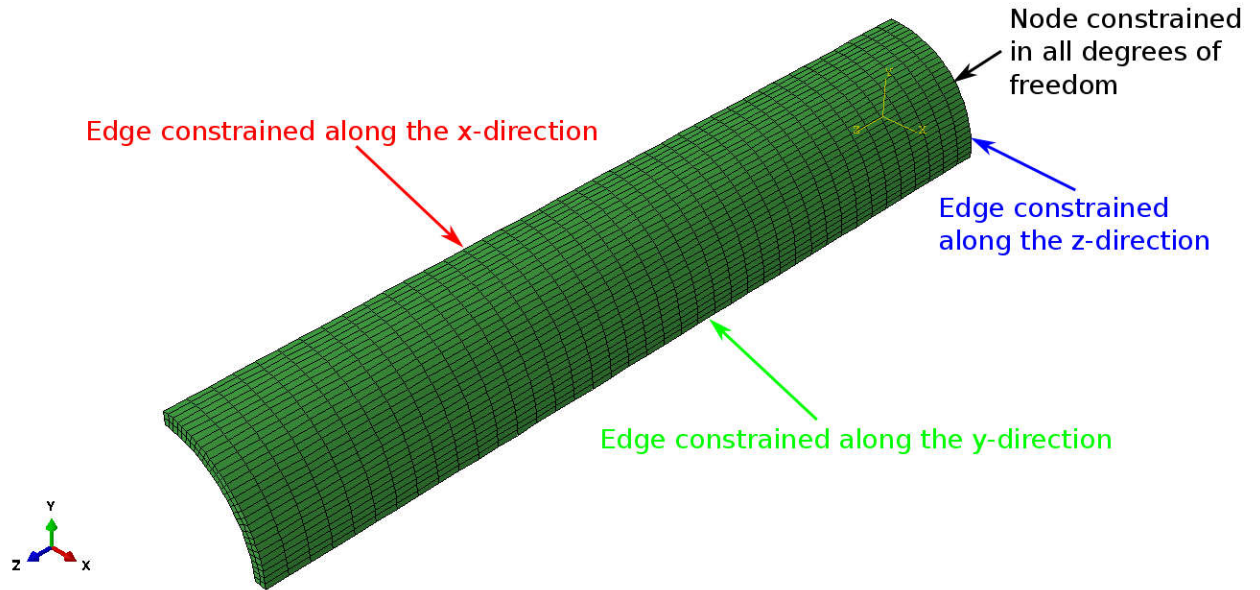


Figure 2. Mesh and boundary conditions for quarter geometry of the cladding tube.

A tube texture representative of a Zircaloy cladding tube was used in the FE simulations. These FE simulations are computationally expensive, especially in terms of the material model calculations. In order to minimize computation costs, a reduced texture comprising of 7 grains is derived from an initial texture comprising of 1144 grains. The Kearn factors for the 7-grain reduced texture are equal to those of the original texture. Pole figures for the reduced texture with 7 grains are shown in Fig. 3. Note that the texture shown in Fig. 3 is the same for every FE element when expressed along the radial, hoop, and axial directions of the cladding tube. However, because the simulation geometry and FE computations are expressed in Laboratory Cartesian coordinates, the texture associated with each element (that is, the constituent crystal orientations) is expressed in Laboratory axes for the Gauss points of each FE.

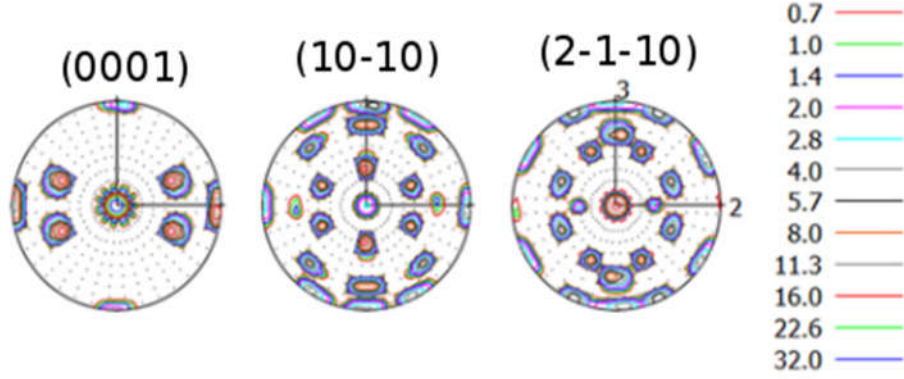


Figure 3. Pole figures for the reduced texture with 7 grains used in the FE simulations. The directions 1, 2, and 3 correspond to the radial, hoop, and axial directions of the cladding tube, respectively.

5.2. Benchmarking VPSC-FE Predictions with VPSC Standalone Predictions

We have performed irradiation growth simulations in both ABAQUS and MOOSE and compared model predictions with standalone VPSC (referred to as VPSC-SA from here on) results for Zircaloy-2. Material parameters calibrated to the experimental growth data for Zircaloy-2 were taken from Ref. [14]. The tube was irradiated at a dose rate of $3.6 \text{ dpa} \cdot \text{s}^{-1}$ to 2 dpa (over 100 time steps) in the absence of external stress.

Figure 4 compares the spatial distribution of strains in the tube from ABAQUS and MOOSE simulations after irradiation to 2 dpa dose. The directions 1, 2, and 3 correspond to the radial, hoop, and axial directions of the cladding tube. The strain concentration near mid-circumference on the right end of the tube is because the mid-circumference node on the right end of the tube is constrained in all degrees of freedom. Moreover, the VPSC-MOOSE simulation shows a more heterogeneous deformation field near the constrained node as compared to the VPSC-ABAQUS simulation, especially for the hoop strain distribution. But apart from that, a fairly homogeneous distribution of strain is predicted along the circumference and the length of the tube, as expected from these irradiation conditions, the symmetry of the tube, and absence of external loading. The tube exhibits negative growth strains along the radial and hoop directions and positive growth strain along the axial direction. This is a consequence of the texture of the tube which has been rolled along the axial direction and is in agreement with experimental evidence of irradiation growth in cold-worked Zircaloy-2 [31].

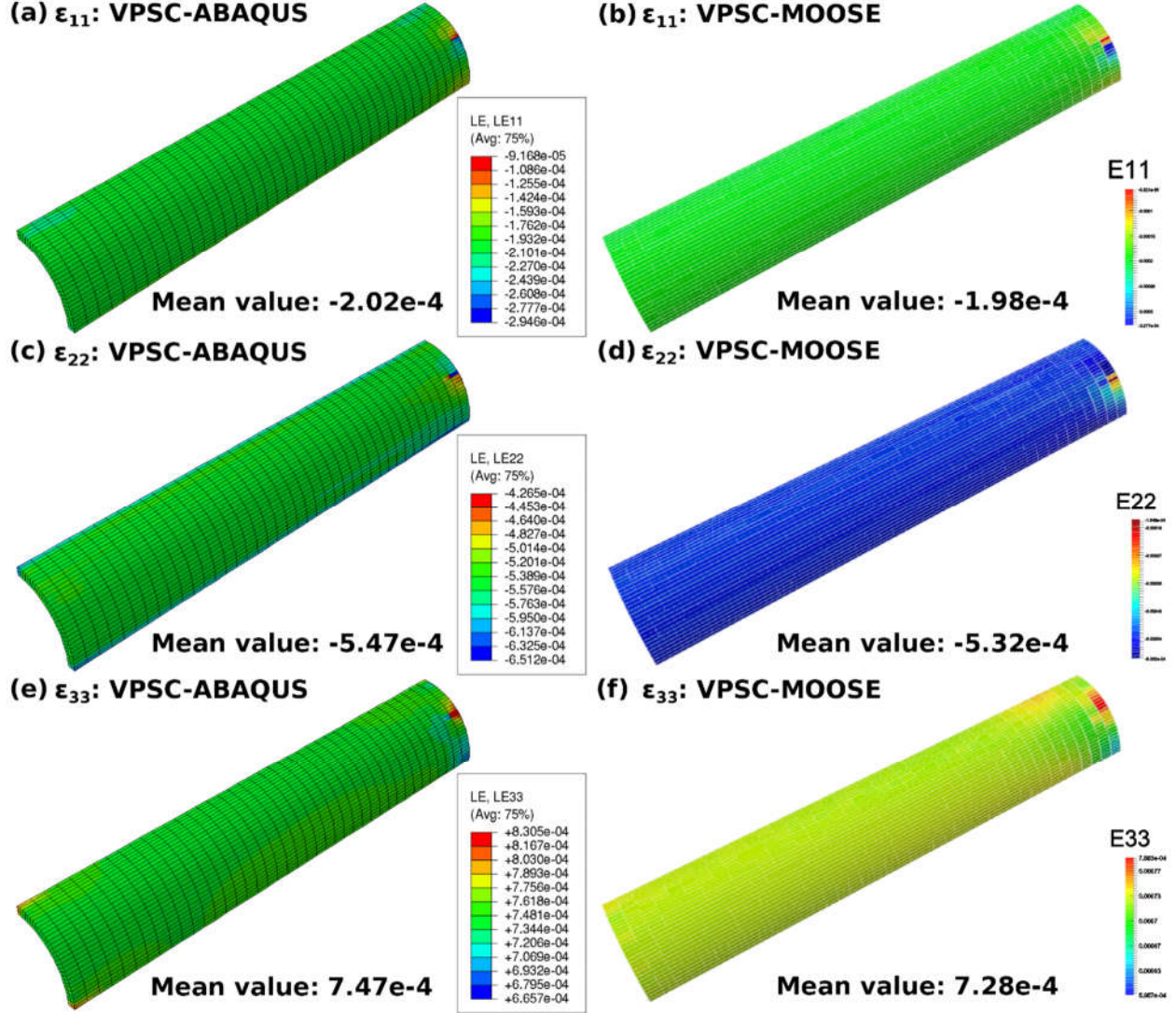


Figure 4. Distribution of (a) radial, (c) hoop, and (e) axial strains from the VPSC-ABAQUS simulation, and (b) radial, (d) hoop, and (f) axial strains from the VPSC-MOOSE simulation after irradiation to 2 dpa dose.

For benchmarking purposes, we picked an element from the middle of the tube mesh and compared the temporal evolution of strains predicted by VPSC-ABAQUS, VPSC-MOOSE, and VPSC-SA. Figure 5 shows the evolution of radial, hoop, and axial strains as a function of radiation dose for the same element. It is seen that predictions from the three simulations are in general agreement. There are some deviations from the VPSC-SA predictions, especially at the beginning, but the predictions appear to converge as one approaches 2 dpa dose. This might be due to the fact that VPSC-SA does not account for elastic deformation, which might be dominant at small strains of about 10^{-4} .

Moreover, there is some difference in model predictions between VPSC-ABAQUS and VPSC-MOOSE. There are two possible reasons for this discrepancy. We have used reduced integration (one integration point per element) FEs in the ABAQUS simulation to minimize computation costs. The MOOSE simulation, on the other hand, uses higher fidelity full integration (eight integration points per element) brick elements. More importantly, we have found that model predictions from MOOSE are dependent on the type of solver used. In the present simulation we used Jacobian-dependent Newton solver option because we found that VPSC-MOOSE predictions deviate significantly from VPSC-SA predictions when using the Pre-Conditioned Jacobian-Free Newton Krylov (PJFNK) solver.

For this benchmark case, the ABAQUS simulation, running on 4 cores (Intel Core i7 3.10 GHz processors) in parallel, was completed in 253 s, while the MOOSE simulation, running on 48 cores (Intel Xeon (Haswell) 2.5 GHz processors) in parallel, was completed in 1049 s. Note that reduced integration FEs were used in ABAQUS, while full integration FEs were used in MOOSE. We plan to perform detailed studies of the effect of different solver types and element types in MOOSE and ABAQUS in order to develop strategies for optimizing the VPSC-FE interface and performance enhancements in future work.

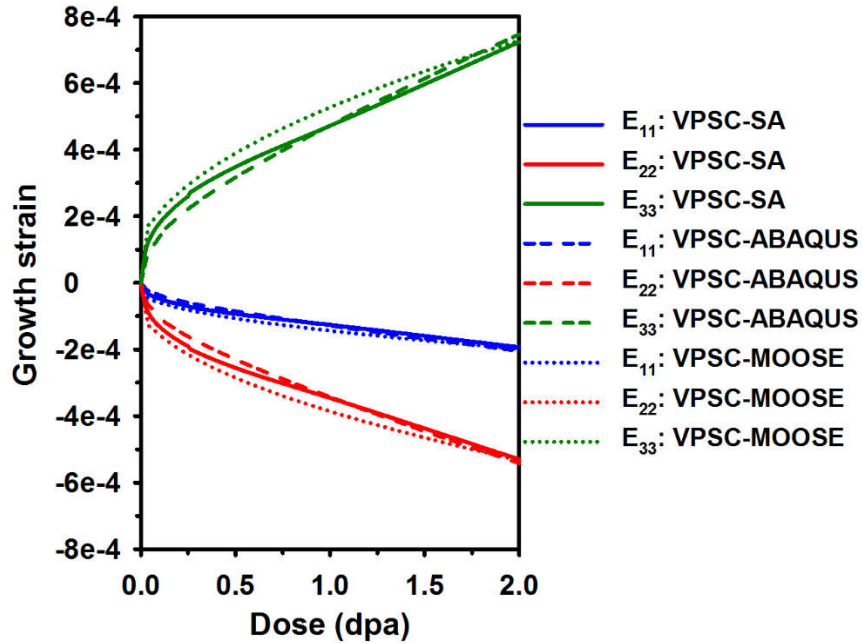


Figure 5. Evolution of growth strains as a function of radiation dose for an element on the circumference on the tube mesh from VPSC-ABAQUS and VPSC-MOOSE simulations as compared to VPSC-SA predictions.

5.3. Effect of Varying the Dose Rate along the Length of the Tube

We performed a simulation where the dose rate was varied along the axis of the tube such that the maximum radiation dose is at one end, and the decay in dose rate follows a Gaussian normal function. The dose rate along the length of the tube is shown in Fig. 6. The irradiation conditions imposed are such that the left (free) end of the tube experiences a total radiation dose of 50 dpa. This simulation is performed using ABAQUS.

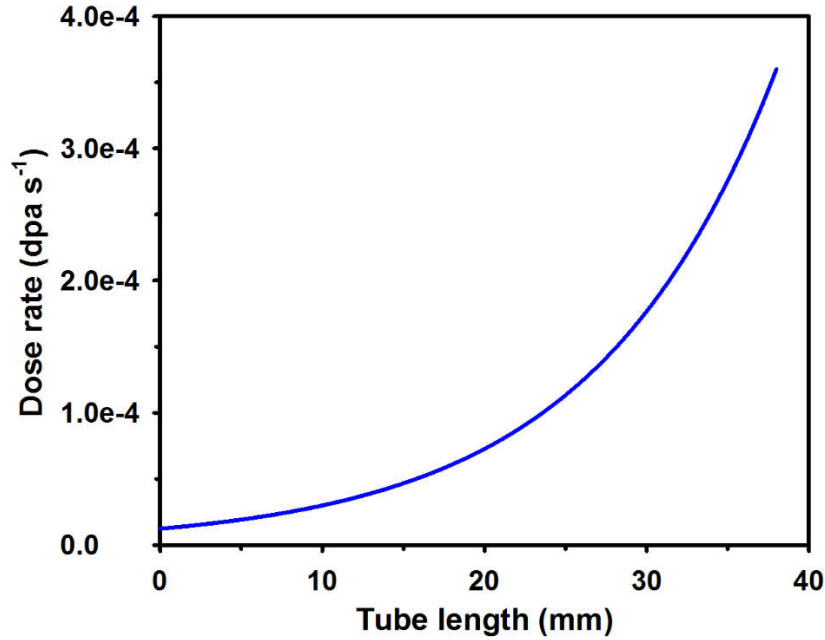


Figure 6. Dose rate along the length of the tube modeled using a Gaussian normal function. 0 mm represents the right (fixed) end of the tube shown in Fig. 2.

The distribution of stress and strain components along the tube is shown in Fig. 7 for these spatially heterogeneous radiation conditions. In all cases, the expected axial symmetry of stress and strain is reasonably predicted, with minor stress concentration near mid-circumference on the left end of the tube and at the position of the fixed element. Those are most likely related to numerical issues. As expected, the axial strain is overall positive and increases gradually from the right to the left end of the tube as the radiation dose rate increases (Fig. 7a). The hoop growth strain, on the other hand, is overall negative and increases as the local radiation dose rate increases. Interestingly, the increasing contraction along the hoop direction induces an interaction between ‘adjacent rings’ and the appearance of a non-zero shear strain ε_{13} . As for the stress components, the axial stress distribution presents tensile stresses in the outer elements of the tube, and compressive stresses in the inner elements (hidden in Fig. 7b). These growth-induced internal stresses trigger irradiation creep in the tube, which in turn relax the stresses. As a result of this auto-catalytic effect, the axial stress does not exceed 20 MPa anywhere. The tendency to contract along the hoop direction

induces an interaction between the outer and inner ring, with the former developing positive and the later negative hoop stress (hidden in Fig. 7d). Once again, irradiation creep keeps these stresses below 25 MPa. The tendency of the tube to contract non-homogeneously along the radial direction induces heterogeneous shear strain ε_{13} (Fig 7c) and an associated shear stress σ_{13} which does not exceed 8 MPa anywhere. Under prolonged irradiation, pressure build-up due to fission gas release, fuel contact, and elevated temperatures occur and these internal stresses may increase and lead to clad failure due to ballooning [32,33].

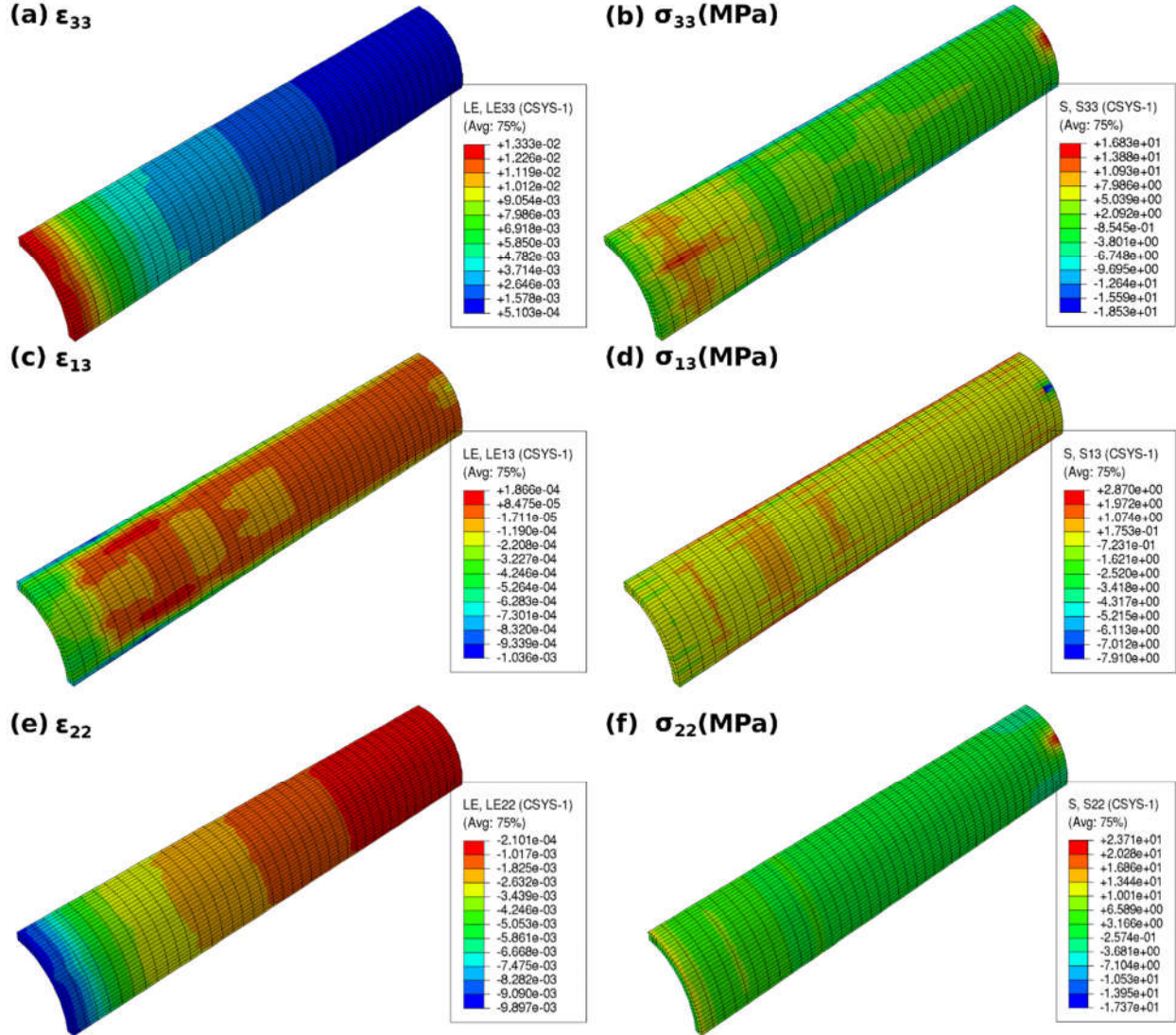


Figure 7. Distribution of (a) axial strain, (b) axial stress, (c) shear (radial-axial) strain, (d) shear (radial-axial) stress, (e) hoop strain, and (f) hoop stress in the tube with a heterogeneous radiation dose history.

6. Summary and Future Work

This Milestone report shows good progress in interfacing VPSC with the FE codes ABAQUS and MOOSE, to perform component-level simulations of irradiation-induced deformation in Zirconium alloys. In this preliminary application, we have performed an irradiation growth simulation in the quarter geometry of a cladding tube. We have benchmarked VPSC-ABAQUS and VPSC-MOOSE predictions with VPSC-SA predictions to verify the accuracy of the VPSC-FE interface. Predictions from the FE simulations are in general agreement with VPSC-SA simulations and also with experimental trends.

In the next phase of this project, the framework will be used to study spacer-clad interactions in a fuel rod assembly, accounting for texture effects and thermo-mechanical effects that contribute to gap opening between the clad and the spacer grid.

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