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THREE-DIMENSIONAL PELLET-CLADDING MECHANICAL INTERACTION THROUGH COHESIVE MODEL IN DIONISIO 3.0

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Abstract. In order to extend the capabilities of the DIONISIO code to three-dimensional domains, we have included a new algorithm to simulate the contact between pellet and cladding and between pellets based in Cohesive Finite Elements. In addition to dividing the rod in a user-defined number of segments, the user can now choose the dimensionality of the domain in which a representative pellet-gap-cladding system is solved. This new model can determine the moment in which two surfaces begin to experience contact and define the evolution of the contact force, including separation of the surfaces and successive contacts. Moreover, it could provide a solution to simulate asymmetric problems concerning the eccentricity of the pellet and cladding, asymmetries in temperature distribution due to the position of a rod in a bundle, especially in accident conditions, or the presence of a defect in the pellet, among others. We present our results testing this kind of contact element, showing improvements over the previous two-dimensional axisymmetric model using Lagrange multipliers and comparing our results with experiments displaying a high correlation so as to validate the concept.

1 INTRODUCTION

1.1 DIONISIO

DIONISIO is a code that simulates most of the phenomena which take place within a fuel rod during irradiation under normal or accident conditions of a nuclear reactor. The code has several tens of interconnected models coupled in a modular structure, predicting thermo-mechanical and thermo-chemical evolution of a fuel rod, thermo-hydraulic behavior of the coolant channel around the rod, plenum temperature variation, liberation of different species generated in the pellet and released to the free volume in the rod, among other processes that can take place in a nuclear fuel rod as fracture and pellet-cladding mechanical interaction (PCMI). The second iteration of DIONISIO has been described in detail in previous papers (Soba and Denis, 2015; Lemes et al. 2015). The finite element method (FEM) is the main numerical tool used to solve the pellet-gap-cladding system. Prior to the incorporation of the three-dimensional models such as the one presented here, axial symmetry was assumed to discretize the domain (Soba and Denis, 2008). This new version of the code allows the user to choose between a two or three-dimensional geometry of said domain. With the objective of better simulating the phenomena involved in a fuel rod, it is partitioned according to user preference. These sections represent portions of the entire rod subjected to different linear power histories, given the nonuniform longitudinal distribution of neutron flux in the reactor and variable boundary conditions. Fig. 1a exhibits an example division of the active portion of an entire fuel rod. In each axial sector representing a given number of pellets, the differential equations (heat, stress, strain) are solved in a representative pellet and the corresponding cladding segment, discretized with hexahedral and pentahedral elements, as shown in Fig. 1b.

In every time step, a complete description of the system variables is obtained for each axial section beginning with the local values of linear power and coolant temperature, followed by the heat diffusion, fission gas release (FGR), swelling, densification, and mechanical equilibrium. Over the material system DIONISIO considers thermal expansion, elastoplastic deformation, creep, densification and swelling (only for the pellet) and irradiation growth (over the Zry cladding) (Soba and Denis, 2015).

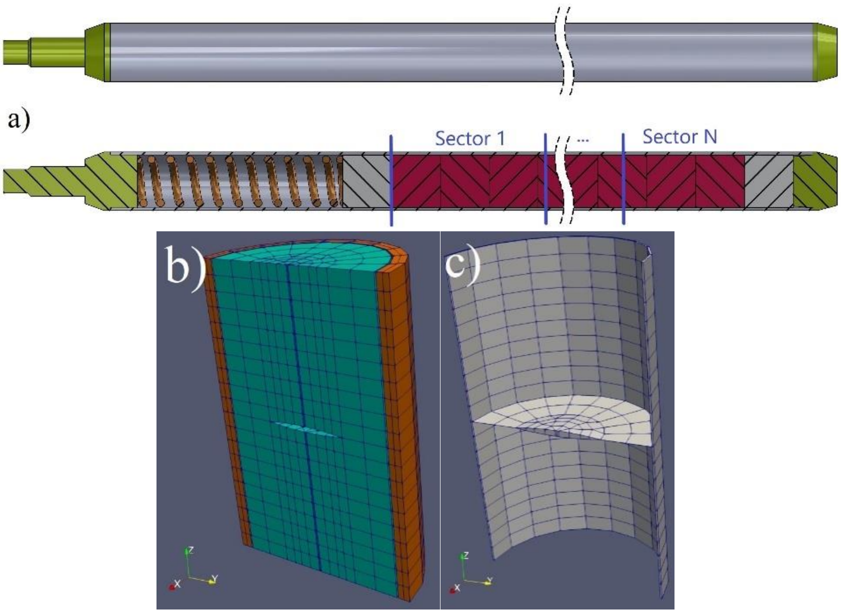

Fig. 1 a) Scheme of an entire rod with several segments, each one containing a number of pellets. b) Two half pellets (green) and cladding (orange). c) Cohesive elements “filling” pellet-cladding and pellet-pellet interfaces.

1.2 PCMI

The mechanical interaction with the pellet is one of the phenomena that report the greatest mechanical demand for the cladding. This phenomenon is induced by a higher temperature in the pellet with a higher thermal expansion and swelling increase, and the concomitant mechanical interaction of the cladding due to creep by the high external pressure. This circumstance is relevant in different instances and under different operating conditions. For low burnup and reactors that operate with collapsible sheath, such as CANDU (Lewis et al. 2009), PCMI is crucial from the first instants of irradiation. In PWR/BWR type reactors, the interaction may occur during the last portion of the life in the reactor (Stimpson et al. 2018), especially during transient power ramps (Herranz et al. 2011). PCMI is also pertinent in high burnup (HB) scenarios, in which fuel contains a significant amount of fission gas atoms in the matrix and gas bubble formation induced by thermally activated diffusion of the gas atoms is capable of causing a considerable magnitude of fuel swelling and PCMI (Suzuki et al. 2004). Similarly, it plays an important role during accident scenarios, especially in reactivity-initiated accident (RIA), (Yueh et al. 2016) when the short power pulses can cause severe damage through this mechanism.

There is a relatively high and continuous production of relevant investigation on this topic (Mathews, 1972; Caillot et al. 1993), and new experiments and simulations provide different points of view and alternative solutions. For example, tests are carried out on systems that emulate PCMI conditions, obtaining data of deformation and hoop stress in idealized situations with high control and ease of measurement. In this type of analysis without irradiation, high power ramps are emulated (Yueh et al. 2016), or fuel pods (both Zry and new materials for accident tolerant fuels) are subjected to the typical stress fields of PCMI (Cazalis et al. 2016; Kim et al. 2009), obtaining valuable data with which it is feasible to validate models and codes.

On the other hand, many more complex tests, generally carried out under irradiation, from which it is more difficult to obtain detailed measurements in situ, are performed continuously in different facilities (Turnbull, 1998; Bruet et al. 1980; Sagrado and Herranz, 2014; Luxat and Novog, 2011).

Finally, some accident tolerant fuel cladding developments need to consider the kind of requirements to which a fuel will be subjected and analyze PCMI during these conditions by performing experiments and numerical simulations of its behavior (Terrani, 2018; Ben-Belgacem et al. 2014).

1.3 DIONISIO 3D

Several fuel codes are devoted to simulating the problem of PCMI, among many other physical-chemical phenomena. Many of them use axial symmetry in the pellet-gap-cladding domain, treating the rod in different heights to contemplate different points of thermo-mechanical interaction (1.5D: Geelhood et al. 2011; Moal et al. 2014; and 2D axisymmetric: Cheon et al. 2004; Linet and Suo, 1993). The use of coupled code systems is quite frequent too, using FEM packages to simulate the thermo-mechanical interaction, linking them to fuel codes.

In the last years, some codes with three-dimensional capabilities have tried to tackle this problem without the use of any symmetry. To name a few, FRAPCON-3.4 developed a 3D module dedicated to PCMI simulation (Kim et al. 2017); the BISON code works in 3D and treats the interaction explicitly (Capps et al. 2017).

While true that two-dimensional approaches respond to most of the thermo-mechanical effects produced by PCMI, they lack the possibility of treating certain asymmetries. The eccentricity of the pellet and cladding, the asymmetry in temperature distribution due to the position of a rod in a bundle, especially in accident conditions, or the presence of a defect in the pellet, among others, are situations in which having a full 3D code could deliver results that better represent the experiments than a two-dimensional one.

In this sense, we have developed version 3.0 of DIONISIO, in which a full 3D plenum description and a new three-dimensional contact algorithm for the pellet-cladding and the pellet-pellet interfaces were included. The contact algorithm, directly related to PCMI, is one of the most complex issues to solve in order to move from the 2D axisymmetric version to an entirely three-dimensional domain. In the previous version of DIONISIO we used the Lagrange multipliers algorithm (Soba and Denis, 2008) which required the assemble of a variable system adding new equations when contact occurs. The added contact equations change the system's matrix properties, making it non-diagonally dominant or non-symmetric if rows are swapped (see second paragraph of section 2). Besides, the error introduced in the successive iterations until reaching convergence, rendered the problem unstable and expensive from a computational point of view. Given this scenario, in the 3D version we have developed an algorithm based on cohesive elements, with a linear contact law that does not alter the system's resolution matrix, making it simpler to solve and easier to parallelize. This method has a notorious disadvantage which is that the problem must be explicitly integrated in time, which is problematic in terms of calculation time involved in comparison to stationary methods (Noels and Radovitzky, 2008). This matter is further discussed at the end of section 2.

In this paper, we present a description of the cohesive element method, its calculation advantages, a few shortcomings and some test results to demonstrate its numerical effectiveness. A tube with an inlaid cylinder test is used to compare the three-dimensional model to other commercial FEM packages and power histories of experiments under irradiation are reproduced, demonstrating its excellent performance compared with the previous version of DIONISIO and experimental results. The last part of the paper presents some brief conclusions.

2 COHESIVE NUMERICAL APPROACH

The PCMI problem in two-dimensional domains in the DIONSIO 2.0 code is treated numerically in the FEM formulation using restriction equations, which do not allow the interpenetration of the surfaces (Soba and Denis, 2008). In each material, an irreducible formulation is applied into the displacement and Lagrange multipliers are used for the treatment of the contact forces over the surface boundaries. The entire formulation is derived from the virtual work principle with the supposition of continuity for the displacement at the frontiers (Gallego and Anza, 1989; Sellgren et al. 2003).

Treating the contact using Lagrange multipliers presents some problems regarding the matrix. Firstly, each new contact pair of contactor-receptor nodes adds n-dimension equations to the system. Secondly, these new rows added to the matrix break the properties of the FEM matrixes, i.e.: they are not diagonally dominant anymore; in fact, each new added row has a zero in the diagonal. Then, new solvers based on biconjugate gradient or similar (Bathe, 2006) need to be applied, using row changes to reorder the system to be solved. These inconveniences escalate when a three-dimensional domain is used, where the finite elements in contact become two-dimensional surfaces. Moreover, the Lagrange multipliers method introduces severe difficulties with respect to the directions of the forces, the slips and tension direction in the transversal and longitudinal directions.

In order to overcome these difficulties, we developed a new method, based in the called cohesive finite elements. The Cohesive Zone concept was initially developed to treat discontinuities that evolve within the continuum, such as cracks, and was conceived by Barenblatt (1962); Dugdale (1960); Rice (1968). These early developments considered the fracture as a gradual phenomenon in which there is a separation between two adjacent virtual surfaces along an extension of the end of the crack (cohesive zone) and is resisted by the presence of cohesive forces. These forces are embodied in tensile-separation laws and link the mechanism of micro structural failure to the deformation field of the continuum. While a conventional crack does not have stress transmission between the corresponding surfaces of the fissure, the "virtual fissure", as it is described by the cohesive zone, is an active field of interactive stress between a pair of virtual surfaces. The fracture process is seen as the progressive decay of the force of the material along adjacent virtual surfaces.

Similarly, but in the opposite direction, a real separation between two surfaces can be treated as a virtual separation. The curve defining the traction-separation involves a particular law that has no effect while the surfaces are separated, determines the moment in which the bodies begin to experience contact and defines the evolution of the contact force in relation to the interpenetration distance (Xu and Needleman, 1994). Considering both normal and tangential traction as linear with respect to interpenetration distance, we can calculate them as follows:

$$T_n = \Phi\delta_n \qquad\qquad T_t = \Phi\delta_t\mu \tag{1}$$

where Φ is obtained from the Young Modulus of the materials, δ_n represents the interpenetration distance, δ_t is the sliding distance (when in contact) and μ is the friction coefficient between both surfaces. The continuous parts of the material are modeled as usual, by classical constitutive equations, for example, Von Mises plasticity with large deformations (Bathe, 2006; Rice, 1968; Xu and Needleman, 1994).

Cohesive elements in contact problems present us with several advantages over the Lagrange multipliers method: no new equations need to be added to the system and the matrices do not lose any of the properties that they have in the FEM; all modifications to the code are introduced when calculating the local contribution of each cohesive element; no new nodes need to be added to the system, since cohesive elements are formed from already existing nodes on the gap boundaries between cladding and fuel pellet or between two pellet surfaces in contact. Lastly, the CZM provides a natural response in case the contact surfaces are separated after contact, and the contact and separation cycle can be performed as many times as necessary.

It is a given that the method possesses some disadvantages. Firstly, the method has severe difficulties for its application in cases where there is large tangential displacement (sliding) between contact surfaces, or the contact pair of element faces is not previously known. As explained in the Introduction, DIONISIO divides the rod in sections and takes a representative pellet for the pellet-gap-cladding system of each sector. The fact that this scenario does not require special studying (as the pellets near the top of the rod would) and the geometry both the pellet and the cladding present, make it a good candidate for the small displacements and small strains consideration, already applied in the previous 2D axisymmetric models, which reduces significantly the possible shortcomings of the method. Another disadvantage of the CZM is the presence of non-physical interpenetration between contact surfaces. Using a dynamic relaxation scheme with pseudo time-stepping (separate from the real time of the power history) provides the possibility to integrate the system explicitly and reach the solution smoothly with the desired precision (Noels and Radovitzky, 2008; Park, 1982; Da Silva et al. 2006). This approach results to be more demanding in terms of calculation time compared to stationary methods, but it allows us to achieve small increments in the displacements, which in turn limit the interpenetration to a minimum (less than 3% of the cladding thickness) while remaining stable and ensuring convergence.

While the method might not be suitable in certain circumstances or for certain specific areas of the rod, we have found that for our simulations the disadvantages of the CZM are far outweighed by the advantages over the Lagrange Multipliers approach.

3 RESULTS

3.1 Contact between tube and inlaid cylinder (Miroliubov et al. 1975)

A problem concerning a solid cylinder of radius r_c with a non-uniform temperature distribution in contact with a tube of internal radius r_c and external radius r_b subjected to an external pressure P_b is analyzed. For a given temperature distribution in the cylinder $T(r)$ an analytical solution for radial displacements of the system is arrived at after numerical integration. The boundary conditions are given by assuming that the solution cannot tend to infinity and considering the stress at the external radius to be equal to the contact pressure

$$u(r) = \frac{\alpha(1+\nu)}{(1-\nu)}\left\{\frac{1}{r}\int_0^r T(r)rdr + \frac{(1-2\nu)r}{r_c^2}\int_0^{r_c} T(r)rdr\right\} - \frac{P_c(1+\nu)(1-2\nu)r}{E} \quad (2)$$

while for the external cylinder the solution is that of a thin tube subjected to an internal pressure P_c and an external pressure P_b. At the point where the contact occurs, the displacement of the cylinder and the tube must be equal, condition from which the expression for the contact pressure of the problem is obtained:

$$P_c = \left(\frac{\frac{\alpha(1+\nu)}{(1-\nu)}\left\{\frac{1}{r}\int_0^r T(r)rdr + \frac{(1-2\nu)r}{r_c^2}\int_0^{r_c} T(r)rdr\right\}\frac{E\left(r_b^2-r_c^2\right)}{r_c} + 2P_b r_b^2}{(1+\nu)(1-2\nu)\left(r_b^2-r_c^2\right)+(1-\nu)r_c^2+(1+\nu)r_b^2}\right) \quad (3)$$

In Fig. 2a, we show the geometry used to solve the problem being a quarter of the tube and cylinder given that the problem is highly symmetric. External pressure is applied on the entire surface of the tube. In Fig. 2b, c, and d, radial and hoop stress along the radius and contact force along the length are shown to correlate very well with results obtained from commercial FEM software COMSOL (https://www.comsol.com, Stockholm, Sweden).

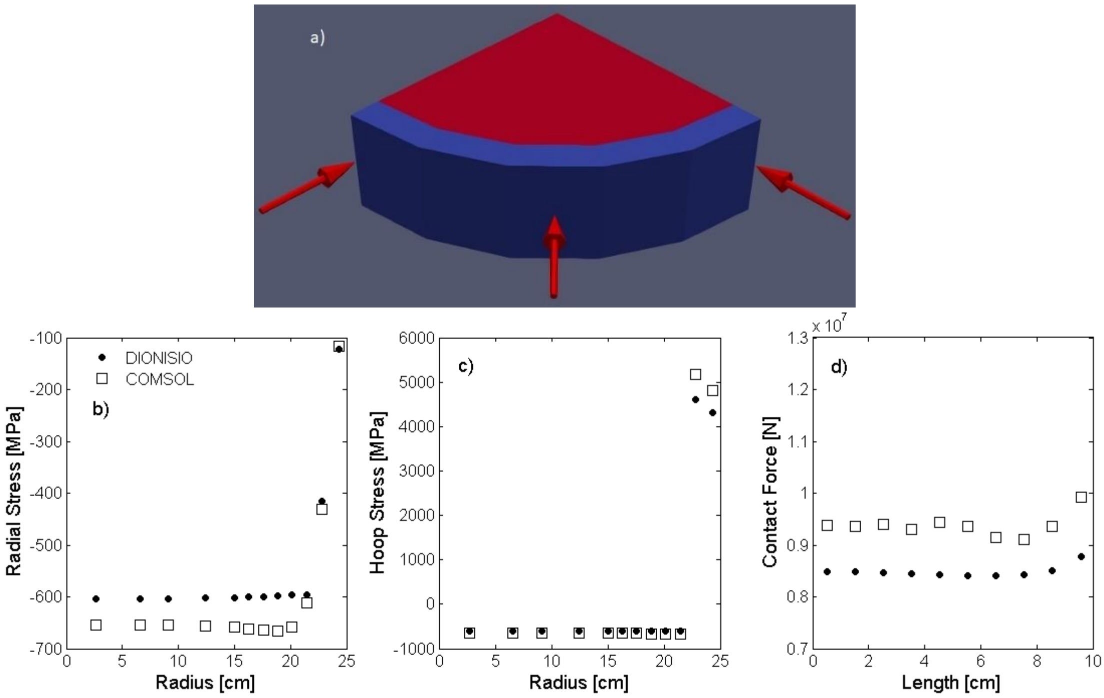

Fig. 2 a) Geometry of tube and inlaid cylinder with external pressure; b) Radial stress along the radius of the domain; c) Hoop stress along the radius of the domain; d) Contact force along the length of the domain. B, c and d are compared to results using COMSOL.

3.2 The Contact Experiment (Turnbull, 1998; Bruet et al. 1980)

The Contact series of experiments used short rods of Zr-4 cladding UO_2 pellets of typical PWR 17x17 design. The purpose of the experiments was to improve the understanding of fuel rod performance. The rods were irradiated in a pressurized water loop at almost constant power and the cladding deformation was measured along other valuable results.

Measurement of cladding diameter for Contact 1 as a function of burnup showed an initial reduction due to creep down followed by a gradual expansion after fuel-to-cladding contact and closed gap. The evolution of diameter versus burnup for Contact 2bis showed an initial increase in diameter over the first 3 cycles of irradiation but there was not an explanation for this increase, as it is followed by a progressive decrease (by irradiation creep) to an equilibrium diameter of approximately 30 microns smaller than the initial.

In general, we can observe a higher power history in Contact 1, which leads to PCMI deforming the cladding with more intensity than Contact 2bis (Fig. 3). The numeric predictions of this experiment are in good correlation to the real values, which have a somewhat considerable dispersion, and prove to be equal to or better than the previous two-dimensional model.

Fig. 4 presents the radius of the cladding (internal) and pellet and the hoop stress as functions of the burnup. In this figure it is possible to see the increase in hoop stress when contact occurs. Some interpenetration can be seen, mainly due to the radii being averages of the circumference and how the CZM performs the numerical solution for contact, as explained in section 2. In Fig. 5, colormaps are shown for distributions of Von Mises stress (left), with radial displacements increased 25 times to make the cladding deformation visible, and temperature (right) for Contact 1. The stress distribution can be seen to decrease radially and axially from the center of the pellet, while the temperature decreases only radially, as is expected.

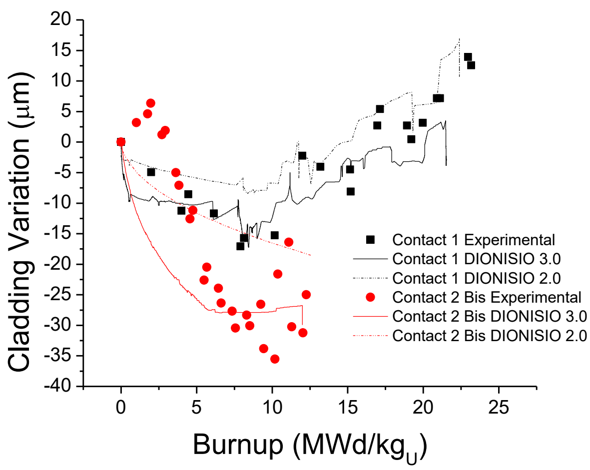

Fig. 3 Cladding deformation through burnup for Contact 1 and Contact 2bis.

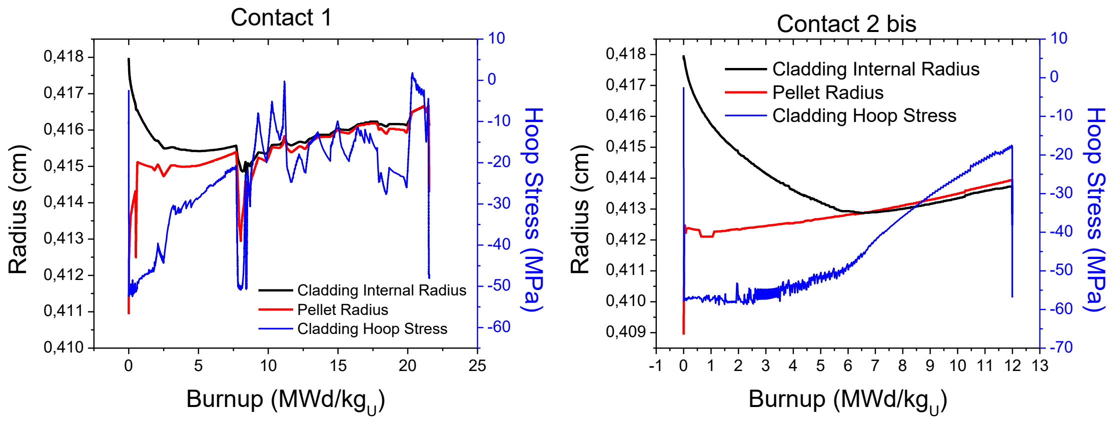

Fig. 4 Evolution of contact surfaces and hoop stress. Left: Contact 1. Right: Contact 2bis.

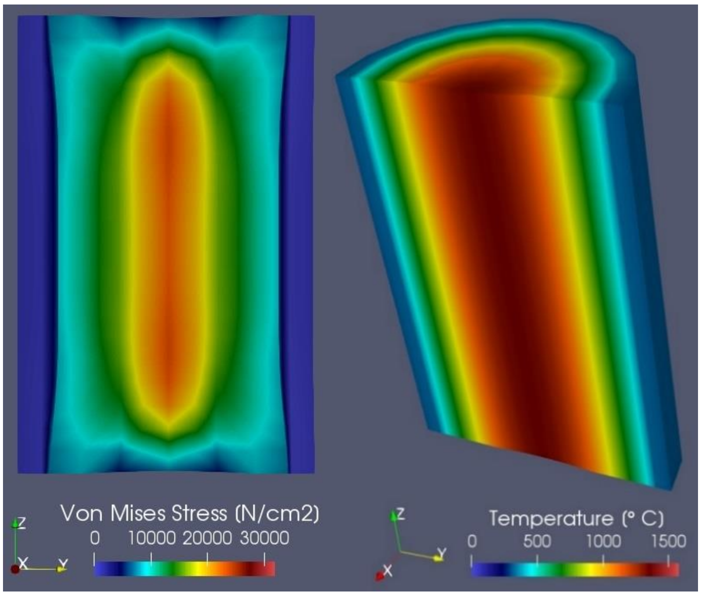

Fig. 5 Contact 1 colormaps. Left: Von Mises stress (radial displacements x25). Right: temperature.

4 CONCLUSIONS

The new three-dimensional model to solve the contact in the pellet-gap-cladding domain by sector is presented. The new algorithm, based in Cohesive Zone methods, a framework included in FEM concepts, developed initially to treat fracture mechanics and problems involving cracks, was necessary for iteration 3.0 of the DIONISIO code to be able to reproduce entire 3D domains. Despite the limitations discussed at the end of section 2, this new contact algorithm shows a better performance in comparison to previously implemented methods regarding scenarios from the literature. Furthermore, we compared the recently incorporated algorithms to experimental tests developed to emulate PCMI with a very good correlation of the results. The use of the algorithm inside the code, considering irradiation and the interplay with the other models included in DIONISIO, exhibits an acceptable performance in the prediction of "bamboo effects" and radial cladding deformation.

In a future publication we will present the general behavior of DIONISIO 3.0, showing the integral performance of the code against complete sets of experimental data to which we have access, so as to validate the complete code in its full three-dimensional version.

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