ADVANCED MECHANICAL RESOLUTION IN CYRANO3 FUEL PERFORMANCE CODE USING MFRONT GENERATION TOOL

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ABSTRACT

The industrial reference software CYRANO3 has been developed by EDF for more than 20 years to simulate the PWR fuel thermo-mechanical behaviour under nominal and incidental conventional operating conditions; CYRANO3 is part of the PLEIADES platform jointly developed by EDF and CEA. Versatility of fuel performance codes, i.e. their ability to cope with various materials, mechanical phenomena or operating conditions, requires support of various mechanical behaviours. The mechanical behaviour integration may have a significant impact on their numerical efficiency. So far, the resolution of the local mechanical constitutive equations in PLEIADES applications required an extensive intrusion into the code structure: this effort had to be done for each mechanical solver used in the platform (CEA applications rely on the Cast3M finite element element solver [13], CYRANO3 uses a specific solver), required much attention to be efficient, and could only be performed by application developers. An open-source code generator named MFRONT was developed in the PLEIADES framework to allow engineers to easily write efficient and reliable mechanical behaviour implementations that can be shared among a wide range of solvers.

The intent of the present contribution is to illustrate the coupling of CYRANO3 and MFRONT-generated libraries in the case of non-linear mechanical constitutive behaviours, such as cladding material viscoplasticity. To this end, a selected example is illustrated step-by-step, based on a cladding creep constitutive model published in the literature.

1. Introduction

The industrial reference software CYRANO3 has been developed by EDF for more than 20 years to simulate the PWR fuel thermo-mechanical behaviour under nominal and incidental conventional operating conditions. The code integrates extensive knowledge and know-how based on more than 30 years of national and international research and feedback in the framework of nuclear materials under irradiation. It is part of the PLEIADES platform jointly developed by EDF and CEA, and validated on an extensive data base including more than 900 irradiated fuel rods examination and validation results.

So far, the resolution of the local mechanical constitutive equations in CYRANO3 was performed thanks to a specific implicit scheme developed and written directly in the kernel of each code. Thus, the implementation of a new constitutive behaviour required an extensive intrusion into the code structure in order to specify the new solving instructions. Additionally, the operation had to be repeated for each new implementation. Those implementations were specific to CYRANO3 and could not be used in other solvers.

To avoid this intrusive and tedious operation, an open-source code generator named MFRONT was developed in the PLEIADES framework [12]. The intent of the present contribution is to illustrate the coupling of CYRANO3 and MFRONT-generated libraries in the case of non-linear mechanical constitutive behaviours, such as cladding material viscoplasticity. To this end, a selected example is illustrated step-by-step, based on a cladding creep constitutive model published in the literature. After writing the model in MFRONT language and generating the associated library, unitary computations of the law as well as a CYRANO3 case study are presented and discussed.

2. A brief overview of CYRANO3 code capabilities

In order to survey the supplier's fuel rod design studies, to establish the operation technical specifications, to build safety studies for new fuel management and to define the initial conditions of accidental situations, EDF needs a reliable way to simulate the PWR thermo-mechanical fuel behaviour. The industrial reference code CYRANO3 has been developed to fulfil these objectives.
The modular architecture of the code is based on a 1D description of the rods using a finite element kernel to solve the thermal and mechanical radial equilibrium at different axial positions. The principle of the geometrical discretisation of a single rod is illustrated in fig.1. Due to revolution axisymmetry, only radial and axial directions are discretised. Further, a simplified generalised plane stress assumption is considered between two axial positions in the rod, leading to the so-called '1,5D' typical axisymmetric scheme composed of different axial slices – each slice being represented by a one-dimensional radial mesh including a pellet and a clad separated by a variable gap. For each element of the meshes, in addition to the thermo-mechanical kernel resolution, different modules allow the computation of thermal, physical and mechanical local properties evolutions with irradiation. The physics of nuclear fuels under irradiation being a strongly coupled problem, an iterative scheme is used to solve the global equations of the rod behaviour including neutronics and thermo-hydraulics simplified correlations, physical-chemical behaviour of the fission products, equilibrium of the clad internal pressure etc. Numerous details of CYRANO3 models have already been regularly published in the literature (e.g. [1] [2] or [3]) and will thus not be recalled in the present article.

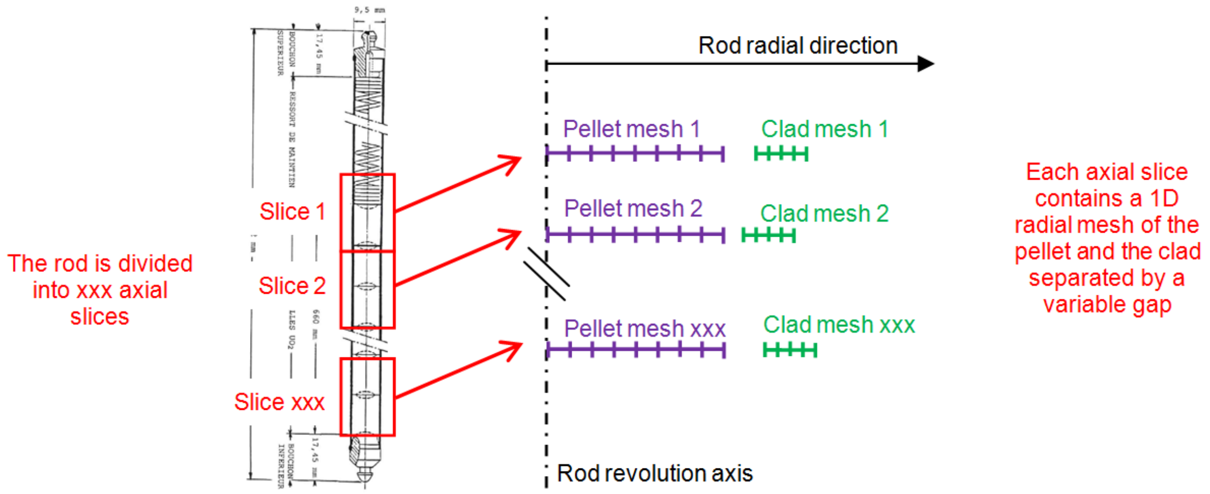

Fig.1: Principle of the rod discretisation in CYRANO3 code

While standard operation of the PWR core (referred to as “class I” condition) is achieved, the fuel rods are submitted to stable and well-calibrated power levels, possibly following slow and restricted variations on a large timescale. During these irradiation cycles, stationary thermal conditions are usually fulfilled. Conversely, hypothetical incidental events (“class II” conditions) may induce fast and extensive power variations of the core, leading to strong evolutive thermal transients in the fuel rods. To account for this wide-ranging variety of solicitations, a static mechanical algorithm is associated with both stationary and transient thermal algorithms in the code. Typical in-core boundary conditions can be considered, such as imposed thermal power level in the pellet with coolant heat exchange on the outer surface of the clad. The temperature can also be imposed directly on the surface of the clad, which leads to a flat temperature radial profile in each axial slice, corresponding to transport/storage typical conditions.

Fuel performance codes accuracy requires a precise and extensive description of the fuel rods materials properties evolutions with irradiation.

Fuel physical models are established on separate parameter measurements (e.g. thermal diffusivity, porosity [4], annealing, sintering, gaseous diffusion…) performed on both fresh and irradiated fuel pellets; a special attention is given to fission gas production and release in the free volumes of the rod, gases production being responsible for the increase of the internal pressure and constituting the major source term in case of accidental failure of the clad. Recently, important progress has been achieved by the introduction in CYRANO3 of a new fission gas prediction module named CARACAS [7], allowing a better description of fission gas production, localisation in the pellet and release during normal and incidental operating conditions. Extensive information about these aspects has been recently published in [8].

Cladding mechanical models are identified by mechanical tests on as-fabricated and irradiated cladding tubes (out and under irradiation). The in-core behaviour of cladding materials can be reproduced and studied in material testing reactors for different fast neutrons flux levels, strain/stress loadings and temperature ranges (e.g. [9]), whereas out-of-core behaviour is mainly characterised in hot cells (for irradiated materials) or conventional labs (non-irradiated) (see for instance [5] or [6]). The main concern regarding cladding mechanical behaviour is related to creep deformation, which can be promoted by both the fast neutrons flux and the temperature. Thus, clad creep models generally dissociate irradiation creep and thermal creep deformation rates. An example of thermal creep law dedicated to the modelling of irradiated cladding materials creep behaviour is detailed in section 4.

Finally, in order to qualify the complete computational and modelling scheme of CYRANO3 code, an integral qualification procedure is systematically applied to validate the code predictions. To this purpose, an extensive validation data base has been constituted on the basis of experimental observations performed on different fuel suppliers’ commercial rods irradiated during survey programs in French and international PWR, as well as rods irradiated in CEA experimental reactors and within the framework of international programs. Thanks to this qualification procedure, predictions of individual models can be compared to their actual experimental values (such as corrosion thicknesses, residual diameters or internal pressures, free volumes etc.), in order to demonstrate the ability of the code to carry out conservative safety studies. The CYRANO3 code therefore integrates extensive knowledge and know-how based on more than 30 years of national and international research and feedback in the framework of nuclear materials under irradiation. It is validated on an extensive data base including more than 900 irradiated fuel rods examination and qualification results.

3. Advanced mechanical resolution in CYRANO3 using MFRONT code generator

3.1. A brief presentation of MFRONT code generator

MFront is a code generator which provides several domain specific languages based on C++ to write mechanical behaviours handling:

- Small and finite strain behaviours, cohesive zone models.
- Isotropic and orthotropic behaviours.
- Various modelling hypotheses: tridimensional, plane strain, plane stress, etc.
- All kind of mechanical phenomena, such as plasticity, viscoplasticity and damage.
- Explicit (Runge-Kutta) and Implicit integration schemes.

Domain specific languages allow the end user to focus on the physics to be treated: specific integration schemes and boilerplate code are automatically generated. Those languages rely on an optimised mathematical library which allows to write constitutive equations in a natural manner.

Various performance assessments, which can be found on the MFront website [12], show that the generated code is on par with native implementations, generally written in fortran. This point is illustrated on Fig.2 in the specific case of the CYRANO3 fuel performance code: comparisons of CPU time on the basis of more than 30 test cases covering a wide range of solicitations show that, on average, MFront implementations are slightly faster than CYRANO3 native implementations. This result is particularly satisfying as the CYRANO3 implementations are based on a much specialised implicit implementation which reduces most mechanical behaviours integration (isotropic or orthotropic) to solving a scalar non-linear equation.

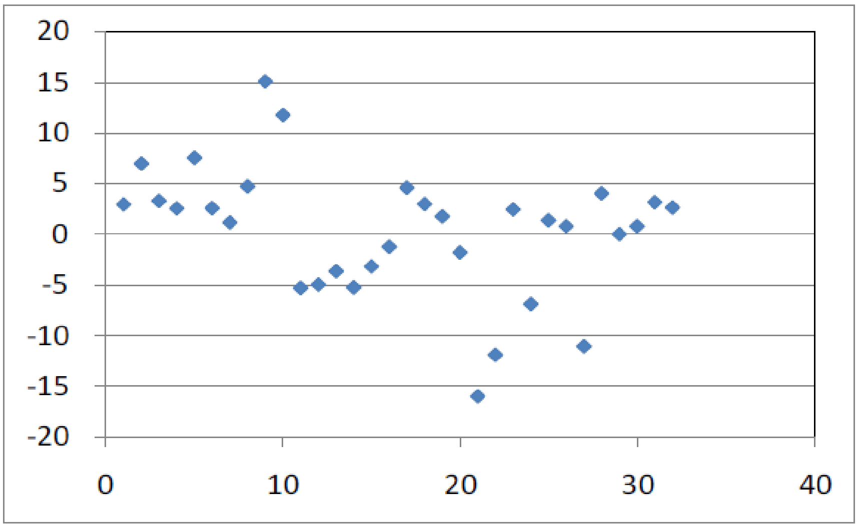

Fig.2: Performance comparison between MFront implementations and native CYRANO3 implementations in various test cases
horiz. axis: relative ratio of the total CPU time in both cases ((MFront-CYRANO3)/CYRANO3*100)
vert. axis: test case number

CYRANO3 aside, MFRONT implementations can be used in various general purpose solvers: Cast3M [13], Code-Aster [14], ZeBuLoN [15]. Support of new solvers, such as EUROPLEXUS [16], is currently considered.

3.2. Using MFRONT-generated code in CYRANO3 local mechanical resolution

Like most finite element solvers, CYRANO3 uses a Newton-Raphson iterative scheme to solve the global mechanical equilibrium over each slice of the rod at every time step; this requires an intermediate resolution stage (often called "local" resolution) consisting in the evaluation of the constitutive behaviour at each Gauss point of the mesh.

Fig. 3 succinctly represents the principle of mechanical equilibrium resolution in CYRANO3. From this very schematic representation, one must essentially note that the local resolution computes stresses and internal variables increments, but also the local consistent tangent operator value, which is of prime importance for the optimal convergence of the global Newton-Raphson scheme.

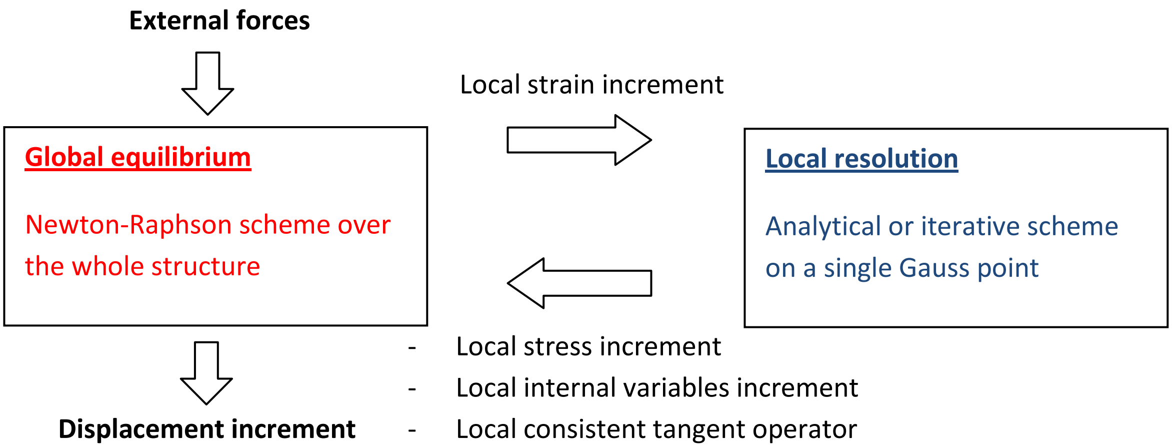

Fig.3: a simplified representation of mechanical equilibrium resolution

Starting from a single set of given constitutive equations, MFRONT translates them into plain C++ instructions embedded in a specific library that allows a full and robust resolution of the differential system. The corresponding library is then linked to the target codes that will share a common optimised implementation of the constitutive behaviour.

Specific developments have thus been recently engaged in CYRANO3 in order to replace the conventional local resolution routines by a new linking process aiming at using MFRONT-generated libraries. The resulting scheme is illustrated on fig.4.

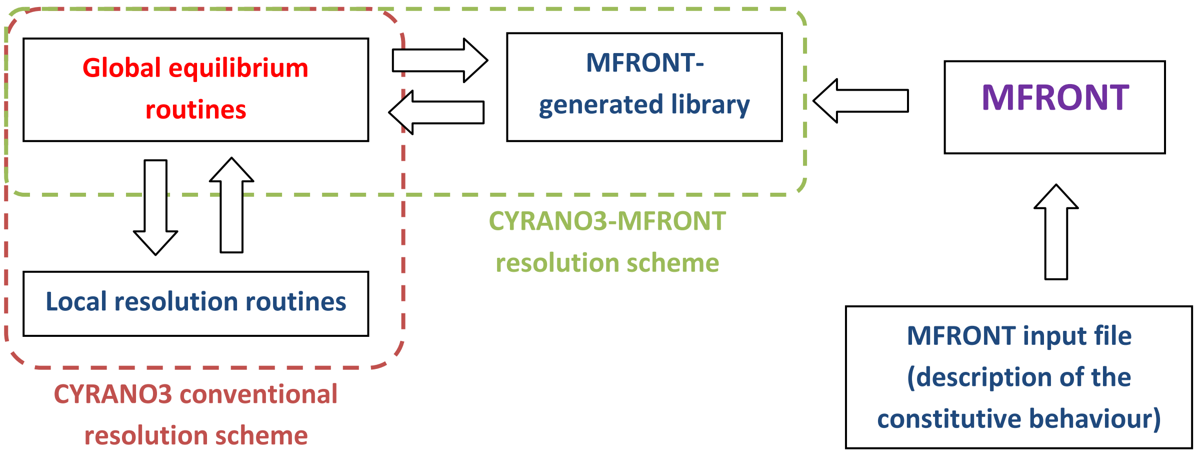

Fig.4: simplified description of the CYRANO3-MFRONT resolution scheme

4. Implementation of a new constitutive law in CYRANO3 using MFRONT

4.1 Description of the law

The selected law has been recently developed and optimised by several authors for the simulation of Zirlo cladding material creep behaviour under wide stress conditions. It is fully described and characterised in different references, such as [9], [10] or [11]. Its main equations are recalled in the followings.

The in-reactor fuel cladding creep is assumed to be a combination of the three following effects: (i) thermal creep, (ii) irradiation-induced deformation and (iii) irradiation hardening effect. The equivalent creep strain ε_{an}^{eq} is expressed as:

$$\varepsilon_{an}^{eq} = \frac{2}{\sqrt{3}}\left[\varepsilon_{sp}\left(1 - e^{-C\sqrt{\dot{\varepsilon}_s t}}\right) + \dot{\varepsilon}_s t\right] \quad (1)$$

With:

$$\varepsilon_{sp} = B\dot{\varepsilon_s}^{b} * [2 - \tanh(D\dot{\varepsilon_s})]^{d} \quad (2)$$

$$\dot{\varepsilon_s} = \frac{AE}{T}e^{-\frac{Q}{RT}}\left[\sinh\left(\frac{2}{\sqrt{3}}a_{irr}\frac{\sigma_{eq}}{E}\right)\right]^{n} + C_0\phi^{C_1}\left(\frac{2}{\sqrt{3}}\sigma_{eq}\right)^{C_2} \quad (3)$$

$$a_{irr} = a[1 - A_1\exp(-A_2\varphi^{A_3})] \quad (4)$$

Where φ (in m^{-2}) stands for the fast neutron fluence, ϕ (in m^{-2}.s^{-1}) the fast neutron flux, σ_{eq} (in Pa) the Von Mises equivalent stress and T (in K) the temperature. Other coefficients are material parameters detailed in [9].

Equation (1) is a time-explicit expression that cannot be considered as a constitutive equation, since it does not involve only thermodynamic forces or dual variables. For a correct implementation in CYRANO3 code, it must be expressed as a deformation rate, i.e. a time-derivative of eq. (1). Considering that expression (1) is valid only for creep tests classical conditions performed at constant stress and temperature levels ($\dot{\sigma_{eq}} = \dot{T} = 0$), and posing $u = \left(1 - e^{-C\sqrt{\dot{\varepsilon}_s t}}\right)$, it is possible to rewrite it as the following time-independent expression:

$$\dot{\varepsilon}_{an}^{eq} = \frac{2}{\sqrt{3}}\left[\varepsilon_{sp}\dot{u} + \dot{\varepsilon_s}\right] \quad (5)$$

With:

$$\dot{u} = -\frac{C^2\dot{\varepsilon_s}}{2.\ln(1-u)}(1 - u) \quad (6)$$

Substituting eq. (5) and (6) to eq. (1) thus allows a complete time-implicit formulation that can be implemented thanks to MFRONT tool.

4.2 MFRONT implementation and validation

For the sake of comparison, two implementations have been performed in MFRONT tool. The first implementation uses a Runge-Kutta explicit iterative resolution scheme, which makes it very simple to write in MFRONT but does not allow for optimal CPU performances. Thus, a second implementation has been developed using Newton-Raphson implicit scheme, in which the exact analytical formulations of the jacobian matrix cross-derivative terms have been calculated and written.

The two versions of the law have then been verified and validated in different conditions.

a. Comparison with an analytical solution

When all the driving variables (i.e. fast neutron flux and fluence, temperature and stress) of the model are supposed constant, eq. (2), (3) and (4) are constant and eq. (5) and (6) integrate in eq. (1) that gives the analytical solution of the problem. This solution can be compared to those calculated by implicit or explicit implementations in MFRONT, as illustrated on fig. 5. In this example, MFRONT solutions have been computed thanks to MTEST software, that allows MFRONT laws simulations on a single material point [17].

Such computations have been performed in different testing conditions, for various stresses, temperatures, fluxes and fluence levels. All the results perfectly fitted the analytical solution. Additionally, it was systematically observed that the implicit integration scheme allowed a considerable computational time reduction, with a variable time reduction factor between 1 and 10.

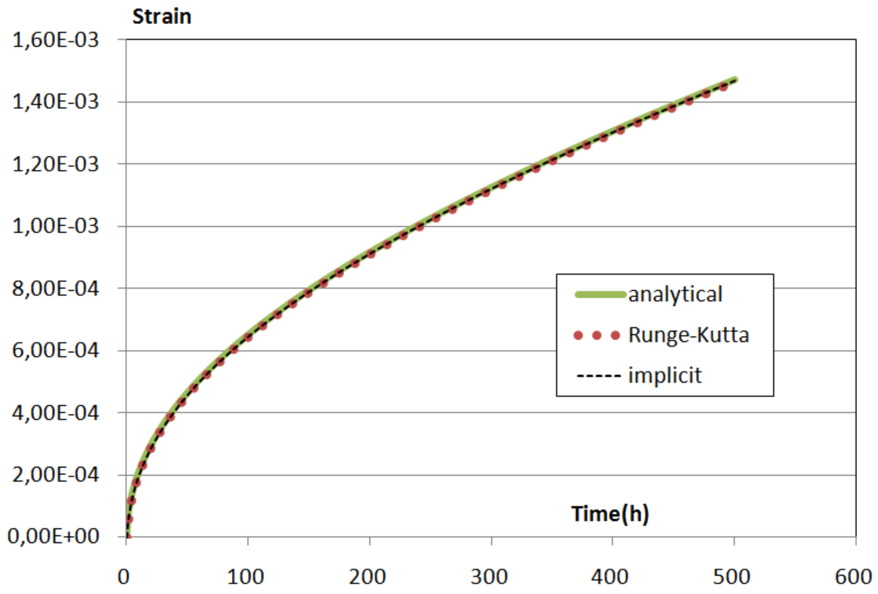

Fig.5: comparison between an analytical solution and MFRONT explicit and implicit implementations

b. Comparison with a reference solution

In [9], the authors compare the results of the model to a set of stress-relaxation tests results performed on irradiated Zirlo samples. In order to simplify the calculations, an approximated version of the model is used considering only the steady-state creep model (i.e. $\dot{\alpha} = 0$ in eq. (6)) and replacing the hyperbolic sine of eq. (3) by an exponential.

We have used the experimental data of [9] and compared them to the results of our MFRONT implementation. The corresponding curves are plotted on fig.6, where single points represent the experimental values collected on XL41, TE1 and XL52 specimens (see [9]), whereas black lines represent the response of the model. For the sake of comparison with [9] calculations, 2 versions of the model have been considered, both respecting the steady-state creep approximation but using either a hyperbolic sine (dotted lines) or an exponential term (solid lines) in eq. (3) flow rule.

From these calculations, we conclude that (i) the results given by our MFRONT implementation are identical to those presented in [9] in the case of the exponential approximation (ii) the replacement of the hyperbolic sine by an exponential is valid for high stress levels, typically above 300MPa for both testing conditions (when doted an plain lines are close to each other). Yet, if long-term low stresses behaviour is to be considered, the exponential approximation leads to a slight under-estimation of eq.(3) real stress level.

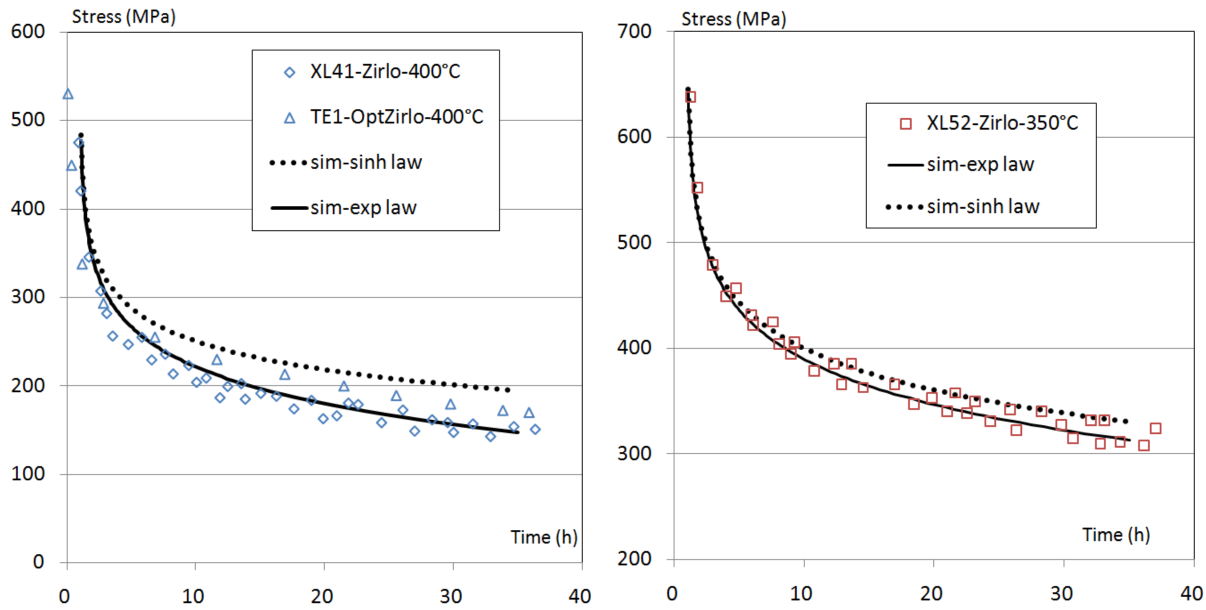

Fig.6: Comparisons between experimental results from [9]
and simulations using different approximations of the creep law

4.3 CYRANO3 case study

The MFRONT implementation of the model was linked to CYRANO3 code, which allowed a complete fuel rod simulation using the new constitutive law. In the followings, we present a some results computed in this framework.

We consider hereafter the following hypothetic case:

- irradiation of a typical PWR UO2/Zirlo rod at 180W/cm up to 35GWd/tM (step 1);
- followed by a 100W/cm/min power ramp up to 350W/cm and 2 hours holding time (step 2).

Such a case loading typically represents severe incidental conditions that can be taken into account in French safety analyses.

For the sake of simplicity, the rod is axially discretised into a single slice (no axial power profile).

Fig.7 presents the evolutions of the rod key mechanical parameters calculated during step 1 phase. Globally, these evolutions obey the following description:

- the differential between primary water loop and rod inner pressure induces a compressive stress state in the cladding, which causes negative creep deformation;
- irradiation creep of the cladding and solid swelling of the pellet promote a progressive closure of the pellet/cladding gap up to 30GWd/tM;
- the compression stress is progressively relaxed by the rod inner pressure increase and the push of the pellet (after gap closure).

Fig.8 presents the evolutions of the rod key mechanical parameters calculated during step 2. From these evolutions, it is very clear that the inner part of the cladding sees the most important solicitation during power ramp loading, which makes it the critical point regarding failure risk analysis. It can also be noted that the evolution of the inner hoop stress during the holding time typically follows the one observed in fig.6, which proves that stress-relaxation tests are particularly appropriate for the study of fuel cladding mechanical resistance under incidental loading conditions.

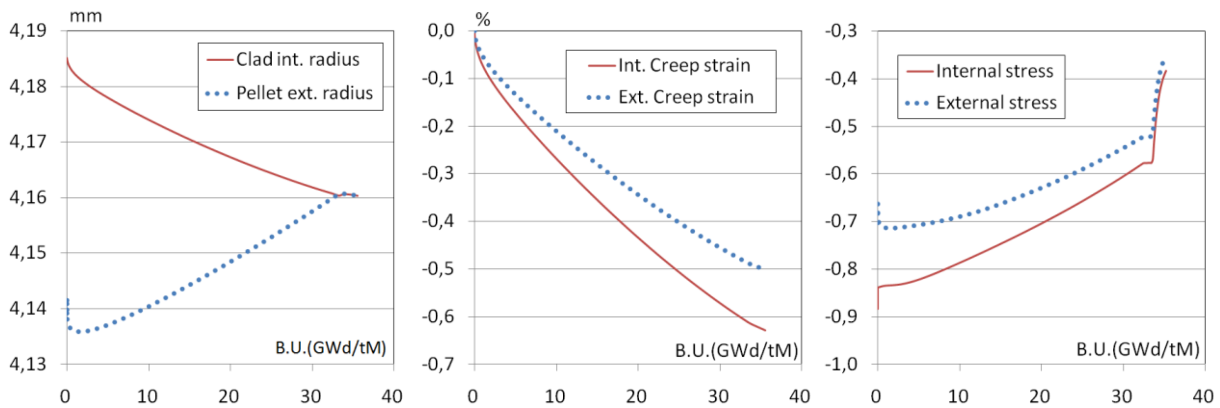

Fig.7: Results of step 1 computation – evolutions as a function of rod burn-up
left: pellet and cladding radii center: cladding inner and outer creep strain
right: cladding inner and outer normalised hoop stresses

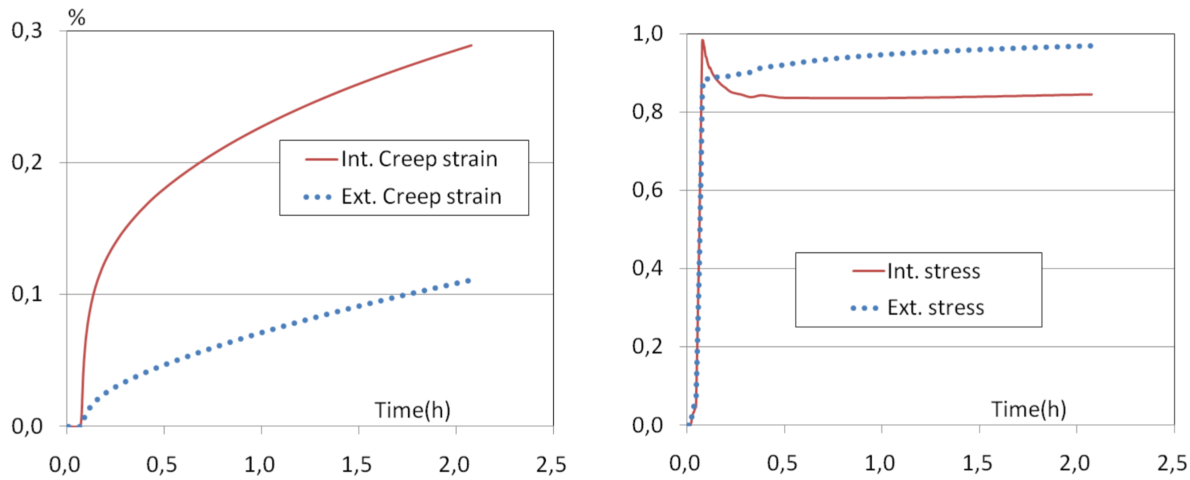

Fig.8: Results of step 2 computation – evolutions as a function of time
left: cladding inner and outer creep strain
right: cladding inner and outer normalised hoop stresses

5. Conclusion

In the present paper, a new feature of EDF fuel performance code CYRANO3 has been considered: the coupling with MFRONT code generator applied to the local resolution of cladding mechanical behaviour. Thanks to this integrated approach, it is possible to implement a single version of a given constitutive behaviour and run it as a standalone model or as part of CYRANO3 code. Such a possibility has been illustrated by the choice, implementation and computation of a cladding creep law from the literature. The presented results show that CYRANO3-MFRONT coupling is a fully effective and versatile implementation solution.

7. Acknowledgements

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