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Extension of monodimensional fuel performance codes to finite strain analysis using a Lagrangian logarithmic strain framework

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HIGHLIGHTS

- A simple extension of standard monodimensional fuel performance codes to finite strain is proposed.
- Efficiency and reliability are demonstrated.
- The logarithmic strain frameword proposed by Miehe et al. is introduced and discussed.

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ABSTRACT

This paper shows how the Lagrangian logarithmic strain framework proposed by Miehe et al. can be used to extend monodimensional fuel performance codes, written in the framework of the infinitesimal strain theory, to be able to cope with large deformation of the cladding, such as the ones observed in reactivity initiated accidents (RIA) or loss-of-coolant accidents (LOCA).

We demonstrate that the changes only concern the mechanical behaviour integration step by a straightforward modification of the strains (inputs) and the stress (result).

The proposed procedure has been implemented in the open-source `MFront` code generator developed within the `PLEIADES` platform to handle mechanical behaviours. Using the `Alcyone` performance code, we apply this procedure to a simulation case proposed within the framework of a recent benchmark on fuel performance codes by the OECD/NEA.

1. Introduction

Normal and typical off-normal operating conditions are well described by fuel performance codes written in the framework of the infinitesimal strain theory (Garcia et al., 2002).

However, reactivity initiated accidents (RIA) or loss-of-coolant accidents (LOCA) induce high mechanical loadings on the fuel rod cladding, leading to large plastic/viscoplastic strains (Fuketa et al., 2001). For example, the mean hoop strain reported for some RIA experiments conducted in Nuclear Safety Research Reactors (NSRR) exceed 10% (Fuketa et al., 1996; Desquines et al., 2011). In some cases, this large strains can lead to the ballooning of the cladding (Flanagan and Askeljung, 2013). A recent benchmark published by the OECD/NEA shows that most fuel performance codes rely on a simplified geometrical representation usually referred to as 1,5D (Committee, 2013). Those fuel performance codes are mostly written using the framework of the infinitesimal strain theory and must be enriched to be able to describe those situations accurately: finite strains must be taken into account (Too and Tamm, 1980; Desquines et al., 2011; Di Marcello et al., 2014).

Di Marcello et al. describes how the `TRANSURANUS` fuel performance code has been extended (Di Marcello et al., 2014). Authors of the recent fuel performance code BISON chose an hypoelastic incremental integration of the material constitutive equations (see Williamson et al., 2012 and the references therein).

The present article describes a solution to take into account the finit strains based on the Lagrangian logarithmic strain framework introduced by Miehe et al. (2002). This framework, whose very appealing features compared to other finite strain framework are described in Section 2, is available in general purpose finite element solvers used by engineers working in the French nuclear energy industry: `Cast3M`, developed by `CEA` (CEA, 2013), `Code_Aster`, developed by `EDF` (EDF, 2013), and `ZeBuLoN`, developed by the Centre des Matériaux de Mines ParisTech as part of the Zset software (Northwest Numerics, 2014). This logarithmic framework has recently been used in the interpretation of compression tests of UO_2 pellets at strain rates similar to those expected during RIA (Salvo et al., 2015). It is therefore very interesting (for consistency) to support this framework in fuel performance codes.

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Table 1
Main notations used in this paper.

$\vec{u}$	Displacement field
$\underset{\sim}{\mathbf{F}} = \underset{\sim}{\mathbf{I}} + \vec{\nabla}\,\vec{u}$	Deformation gradient
$J = \det\left(\underset{\sim}{\mathbf{F}}\right)$	Volume change
Strain tensors	
$\underline{\mathbf{C}} = {}^t\underset{\sim}{\mathbf{F}}\cdot\underset{\sim}{\mathbf{F}}$	Right Cauchy tensor
$\underline{\mathbf{U}} = \underline{\mathbf{C}}^{1/2}$	Stretch tensor
$\underset{\sim}{\epsilon}^{to}_{HPP} = \frac{1}{2}\left(\vec{\nabla}\,\vec{u} + {}^t\vec{\nabla}\,\vec{u}\right)$	Linearised strain tensor
$\underset{\sim}{\epsilon}^{to}_{log} = \log\left(\underset{\sim}{\mathbf{U}}\right)$	Hencky strain tensor
$\underset{\sim}{\epsilon}^{to}_{GL} = \frac{1}{2}\left(\underline{\mathbf{C}} - \underline{\mathbf{I}}\right)$	Green–Lagrange strain
Stress tensors	
$\underset{\sim}{\mathbf{P}}$	First Piola–Kirchhoff stress
$\underline{\mathbf{S}}$	Second Piola–Kirchhoff stress
$\underline{\boldsymbol{\tau}}$	Kirchhoff stress
$\underline{\boldsymbol{\sigma}}$	Cauchy stress

We demonstrate in Section 3, which is the core of this paper, that the extension of fuel monodimensional performance codes written in the framework of the infinitesimal strain theory can be straightforward. This extension is limited to a pre- and post-processing of the behaviour integration step: no change is required in the algorithms used to solve the mechanical equilibrium. The accuracy and the robustness of the proposed extension is checked on some unit tests by comparison to analytical results or various multi-dimensional computations performed using the `Cast3M` finite element solver (CEA, 2013).

The main target of this work is the `Alcyone` fuel performance code developed within the `PLEIADES` platform (Plancq et al., 2004) which uses the `Cast3M` finite element solver to perform thermo-mechanical simulations. Mechanical behaviour implementations were made using the `PLEIADES MFront` code generator (CEA, 2014). The extension proposed in this paper is applied to a simulation proposed by the OECD/NEA in a recent benchmark (Committee, 2013).

The main notations used in this paper are reported in Table 1.

2. General description of the logarithmic strain framework

In this section, we recall some basic definitions used in finite strain structural mechanics, the main results obtained by Miehe et al. (2002) and emphasise the main advantages of the logarithmic strain framework.

2.1. Kinematics

The deformation $\vec{\phi}$ relates the position $\vec{X}$ of a point in the reference configuration Ω_0 and its position $\vec{x}$ in the current configuration Ω_t:

$$\vec{x} = \vec{\phi}(\vec{X}) \tag{1}$$

The displacement $\vec{u}$ is the difference between $\vec{x}$ and $\vec{X}$:

$$\vec{u} = \vec{x} - \vec{X} = \vec{\phi}(\vec{X}) - \vec{X} \tag{2}$$

The deformation gradient $\underset{\sim}{\mathbf{F}}$ is related to the gradient of the displacement:

$$\underset{\sim}{\mathbf{F}} = \frac{\partial\vec{\phi}}{\partial\vec{X}} = \underset{\sim}{\mathbf{I}} + \vec{\nabla}\,\vec{u} \tag{3}$$

$\underset{\sim}{\mathbf{F}}$ can be expressed by the product of a rotation $\underset{\sim}{\mathbf{R}}$ and a stretch tensor $\underline{\mathbf{U}}$:

$$\underset{\sim}{\mathbf{F}} = \underset{\sim}{\mathbf{R}}\cdot\underline{\mathbf{U}} \tag{4}$$

This polar decomposition is unique.

The infinitesimal strain tensor $\underset{\sim}{\epsilon}^{to}_{HPP}$ is defined by:

$$\underset{\sim}{\epsilon}^{to}_{HPP} = \frac{1}{2}\left(\vec{\nabla}\,\vec{u} + {}^t\vec{\nabla}\,\vec{u}\right) = \frac{1}{2}\left(\underset{\sim}{\mathbf{F}} + {}^t\underset{\sim}{\mathbf{F}}\right) - \underline{\mathbf{I}} \tag{5}$$

2.2. Lagrangian strain tensors

An infinite number of strain tensors can be build using the stretch tensor $\underline{\mathbf{U}}$. Only two will be considered in this paper:

- The Green–Lagrange tensor $\underset{\sim}{\epsilon}^{to}_{GL}$:

$$\underset{\sim}{\epsilon}^{to}_{GL} = \frac{1}{2}\left(\underline{\mathbf{U}}^2 - \underline{\mathbf{I}}\right) = \frac{1}{2}\left(\underline{\mathbf{C}} - \underline{\mathbf{I}}\right) \tag{6}$$

- The Hencky strain tensor $\underset{\sim}{\epsilon}^{to}_{log}$:

$$\underset{\sim}{\epsilon}^{to}_{log} = \log\underline{\mathbf{U}} = \frac{1}{2}\log\underline{\mathbf{C}} \tag{7}$$

where $\underline{\mathbf{C}} = {}^t\underset{\sim}{\mathbf{F}}\cdot\underset{\sim}{\mathbf{F}}$ is the right Cauchy tensor.

The volume expansion, measured by the determinant of the deformation gradient, is directly linked to the trace of the Hencky strain tensor:

$$J = \det\left(\underset{\sim}{\mathbf{F}}\right) = \exp\left(\mathrm{tr}\ \ \underset{\sim}{\epsilon}^{to}_{log}\right) \tag{8}$$

2.3. Equilibrium

Mechanical equilibrium in the current configuration Ω_t is given by:

$$\vec{\nabla}_{\vec{x}}\cdot\underline{\boldsymbol{\sigma}} = 0 \tag{9}$$

where $\underline{\boldsymbol{\sigma}}$ is the Cauchy stress tensor. Equilibrium in the initial configuration Ω_0 is given by:

$$\vec{\nabla}_{\vec{X}}\cdot\underset{\sim}{\mathbf{P}} = 0 \tag{10}$$

where $\underset{\sim}{\mathbf{P}}$ is the first Piola–Kirchhoff stress.

Boundary conditions The first Piola–Kirchhoff stress satisfies the following boundary condition:

$$\mathrm{d}\vec{f} = \underset{\sim}{\mathbf{P}}\cdot\mathrm{d}S\,\vec{N} \tag{11}$$

where $\mathrm{d}S$ is an infinitesimal surface oriented by the outer normal to the body $\vec{N}$ in the reference configuration and where $\mathrm{d}\vec{f}$ is the force in the current (deformed) configuration acting on the image $\mathrm{d}s$ of $\mathrm{d}S$.

2.4. Energetic conjugates

A strain tensor and a stress tensor are conjugated when the contracted product of this strain rate and of this stress is equal to the mechanical power p in the initial configuration (see Eq. (12)). For example, the Green–Lagrange strain is the conjugate of the second Piola–Kirchhoff stress $\underline{\mathbf{S}}$.

The key idea of Miehe et al. approach was to define a new stress tensor $\underline{\mathbf{T}}$ as the conjugate of the rate of the Hencky strain tensor (Miehe et al., 2002). $\underline{\mathbf{T}}$ thus satisfies the following equation:

$$p = \frac{1}{J}\underline{\boldsymbol{\sigma}} : \underline{\mathbf{D}} = \underline{\boldsymbol{\tau}} : \underline{\mathbf{D}} = \underline{\mathbf{T}} : \dot{\overline{\epsilon}}^{to}_{\log} = \underset{\sim}{\mathbf{P}} : \dot{\mathrm{F}} = \underline{\mathbf{S}} : \dot{\overline{\epsilon}}^{to}_{GL} = \frac{1}{2}\underline{\mathbf{S}} : \dot{\mathbf{C}} \tag{12}$$

where $\underline{\boldsymbol{\tau}}$ is the Kirchhoff stress, $\underline{\mathbf{D}}$ the deformation rate. An explicit link between $\underline{\mathbf{T}}$ and the Piola–Kirchhoff stresses $\underline{\mathbf{P}}$ and $\underline{\mathbf{S}}$ can be derived from Eq. (12):

$$\underline{\mathbf{P}} = \underline{\mathbf{T}}.\frac{\partial\underset{\sim}{\epsilon}^{to}_{log}}{\partial\underline{\mathbf{F}}} \quad \text{and} \quad \underline{\mathbf{S}} = 2\,\underline{\mathbf{T}}.\frac{\partial\underset{\sim}{\epsilon}^{to}_{log}}{\partial\underline{\mathbf{C}}} \tag{13}$$