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Implicit integration of the constitutive equations of a polycrystal obtained by the Berveiller-Zaoui homogeneization scheme

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Abstract — This paper shows how to integrate polycristal behaviours obtained by the Berveiller-Zaoui homogeneization scheme (1) using an implicit integration scheme. Such polycristalline behaviours require special care as the number of internal state variables can be very high: typically several hundred state variables may be involved.

In the literature, explicit schemes are therefore classically used. To the best of our knowledge, the presented implicit scheme is original and is made feasible by the use of a static condensation of the internal state variables associated with each phase, the implementation of which is involved.

The presented implicit scheme may considerably reduce the computation efforts at the global scale by providing the consistent tangent operator. The latter point may allow widespread use of such models in large scale structural computations in standard finite element solver.

An application to zirconium alloys is used as an illustrative example following the work of Onimus et al (2).

1 Introduction

The aim of this contribution is to describe briefly the implementation of a simple self-consistent polycrystalline model based on the use of the Berveiller-Zaoui concentration rule (1).

In this work, a phase is defined as a set of grains having the same crystallographic orientation.

This model provides an explicit relationship between the stress average over a given crystallographic phase, and the macroscopic applied stress. This model assumes both an isotropic elastic behaviour and isotropic plastic behaviour at the macroscopic scale.

1.1 Outline

After a quick recall of the equations involved in Section 2, we describe in depth how to integrate such behaviour using an implicit scheme.

Implicit schemes for the integration of polycrystal behaviours obtained by homogeneization have been studied in previous works, see (3, 4) for example. However, those methods do not guarantee a quadratic convergence locally (at the integration point scale) nor provide an exact consistent tangent operator which guarantee a quadratic convergence of the equilibrium at the structural scale.

The proposed integration scheme is, to the best of our knowledge, original. This scheme is based on a special choice of the integration variables and a static condensation technique to eliminate the internal state variables of the crystallographic phases.

It is shown that this implementation is locally quadratically convergent and, since it provides an exact tangent operator, quadratically convergent at the structural scale.

The latter point may allow the widespread use of such models in large scale structural computations. Moreover, this scheme is easily adaptable for complex local behaviours of the phases and/or other homogeneization schemes.

1.2 Notations

- $\underline{\Sigma}$: the macroscopic stress.
- Σ_{eq}: the macroscropic von Mises stress.
- $\underline{E}^{\text{to}}$: the macroscopic strain.
- $\underline{E}^{\text{vp}}$: the macroscopic viscoplastic strain.
- N_g: number of grains/phases.
- $\underline{\sigma}^{(k)}$: the stress average over the k$^{\text{th}}$ phase.
- $\phi^{(k)}$: the volume fraction of the k$^{\text{th}}$ phase:

$$\phi^{(k)} = \frac{V^{(k)}}{\sum_{l=1}^{N_g} V^{(l)}}$$

- M: the macroscropic shear modulus.
- N_ν: the macroscropic Poisson ratio.
- P: the equivalent macroscopic viscoplastic strain.
- $g^{(k,i)}$: average plastic slip along the i$^{\text{th}}$ slip system of the k$^{\text{th}}$ phase.
- $\mu^{(k,i)}$: orientation tensor of the i$^{\text{th}}$ slip system of the k$^{\text{th}}$ phase.

2 Constitutive equations

2.1 The Berveiller-Zaoui homogeneization scheme

In the framework of macroscopically isotropic elasto-plastic behaviors, Berveiller and Zaoui have derived a self-consistent polycrystalline model using a secant approximation for the linearization of the non-linear behavior of materials (1). The grains of the polycrystal have equiaxed shape and the texture of the material is isotropic. The local elasticity is assumed homogeneous and isotropic. In the case of monotonous radial loadings Berveiller and Zaoui have shown that the stress average $\underline{\sigma}^{(k)}$ over a crystallographic phase (k) can be expressed explicitly as a function of the local plastic strain $\underline{\varepsilon}^{\text{vp}(k)}$, the macroscopic stress $\underline{\Sigma}$ and the macroscopic viscoplastic strain $\underline{E}^{\text{vp}}$.

The macroscopic strain $\underline{E}^{\text{to}}$ is split additively in a macroscopic elastic part $\underline{E}^{\text{el}}$ and a macroscopic viscoplastic strain $\underline{E}^{\text{vp}}$:

$$\underline{E}^{\text{to}} = \underline{E}^{\text{el}} + \underline{E}^{\text{vp}} \tag{1}$$

The macroscopic stress $\underline{\Sigma}$ is related to the macroscopic elastic strain $\underline{E}^{\text{el}}$ by the Hooke law:

$$\underline{\Sigma} = \underline{D} : \underline{E}^{\text{el}} \tag{2}$$

where $\underline{D}$ is an elastic isotropic macroscopic stiffness that can be expressed using the macroscopic shear modulus M and the macroscopic Poisson ratio N_ν.

The macrosopic viscoplastic strain is linked to the average plastic strain $\underline{\varepsilon}^{\text{vp}(k)}$ by a simple mixing rule:

$$\underline{E}^{\mathrm{vp}} = \sum_{k=1}^{N_g} \phi^{(k)}\, \underline{\varepsilon}^{\mathrm{vp}(k)} \tag{3}$$

where $\phi^{(k)}$ is the volume fraction of the k$^{\mathrm{th}}$ phase.

The local stress $\underline{\sigma}^{(k)}$ is given by the following relationship[1]:

$$\underline{\sigma}^{(k)} = \underline{\Sigma} + 2\,M\alpha(\Sigma_{\mathrm{eq}}, P)\,(1-\beta(N_\nu))\left(\underline{E}^{\mathrm{vp}} - \underline{\varepsilon}^{\mathrm{vp}(k)}\right) \quad \text{with} \quad \beta(N_\nu) = \frac{2}{15}\,\frac{4-5\,N_\nu}{1-N_\nu} \tag{4}$$

where:

- Σ_{eq} is the macroscropic von Mises stress.
- P is the equivalent macroscropic viscoplastic strain defined in an incremental way as follows:

$$\dot{P} = \sqrt{\frac{2}{3}\,\dot{\underline{E}}^{\mathrm{vp}} : \dot{\underline{E}}^{\mathrm{vp}}}$$

  with 0 as the initial value.

The function $\alpha(\Sigma_{\mathrm{eq}}, P)$ is called the accommodation function. It represents the plastic accommodation between the Homogeneous Equivalent Medium and the considered crystallographic phase (r) in inclusion (spherical inclusion). The expression of the accommodation function is as follows:

$$\alpha(\Sigma_{\mathrm{eq}}, P) = \frac{2\,\Sigma_{\mathrm{eq}}}{2\,\Sigma_{\mathrm{eq}} + 3\,M\,P}$$

Equations (3) and (4) are important as they summarize the Berveiller-Zaoui homogeneization scheme, i.e. how the macroscopic and microscopic aspects are coupled. Equation (4) will be the basis of the static condensation method used to build the implicit scheme presented in Section 3 because it shows that the average stress $\underline{\sigma}^{(k)}$ only depends on the macroscopic variables $\underline{\Sigma}$ and $\underline{E}^{\mathrm{vp}}$ and the viscoplastic strain $\underline{\varepsilon}^{\mathrm{vp}(k)}$ of the considered phase.

Using this explicit concentration rule, it is particularly simple to compute the overall response of a polycrystalline material, provided the intra-granular constitutive behaviour is known.

2.2 Intra-granular constitutive behavior

In this report, we assume that the local constitutive equations have the following form:

$$\dot{\underline{\varepsilon}}^{\mathrm{vp}(k)} = v^{(k)}\left(\underline{\sigma}^{(k)}\right) \tag{5}$$

where the microscopic plastic strain may results from the slips along the slip systems of the crystal following:

$$\dot{\underline{\varepsilon}}^{\mathrm{vp}(k)} = \sum_{i=1}^{N_s} \dot{g}^{(k,i)}\,\mu^{(k,i)} \quad \text{with} \quad \dot{g}^{(k,i)} = \left\langle \frac{\sigma^{(k)} : \mu^{(k,i)} - R_0}{K} \right\rangle^n$$

[1] The $\beta(N_\nu)$ factor is closed to $\frac{1}{2}$ for a macroscopic Poisson ratio close to 0.3. In this case, the Localisation Equation (4) may be simplified as:

$$\underline{\sigma}^{(k)} = \underline{\Sigma} + M\alpha(\Sigma_{\mathrm{eq}}, P)\left(\underline{E}^{\mathrm{vp}} - \underline{\varepsilon}^{\mathrm{vp}(k)}\right)$$

This constitutive equation is very simple, but extensions of the proposed integration scheme to more complex ones, such as i.e. the Méric-Cailletaud behaviour (5), is straightforward using an explicit scheme and feasible for the implicit scheme although more involved.

For the example, we will follow the work of Onimus et al. with sightly modified material coefficients (2).

3 Implicit integration scheme

3.1 Former implicit integration schemes

Following the implicit integration scheme proposed in the past (see (3)), the set of integration variables are the averages per phase of the stress field, namely the N_g symmetric second-order tensors $\underline{\sigma}^{(k)}$. These N_g unknowns are the solutions of the N_g system of equation (4), where $\underline{E}^{vp}$ and $\underline{\epsilon}^{vp(k)}$ can be expressed as a function of these unknowns (relations (3) and (5), respectively) while $\underline{\Sigma}$ is obtained from:

$$\underline{\Sigma} = \sum_{k=1}^{N_g} \phi^{(k)} \, \underline{\sigma}^{(k)} \tag{6}$$

The size of the resulting system of nonlinear equations equals $6\,N_g \times 6\,N_g$ which makes difficult its resolution with the Newton-Raphson method. As a result, (3) proposed to solve this nonlinear system of equations with a fixed-point iterative method : for a given trial set of the unknowns, the macroscopic stress $\underline{\Sigma}$ and viscoplastic strain $\underline{E}^{\mathrm{vp}}$ are computed from Equations (3) and (6). Next, for each phase (k), as the average viscoplastic strain in a given phase (k) is a function of the average stress (Equation (5)) in the same phase, the N_g relations (4) are solved separately by a Newton-Raphson method. A new set of the average stresses per phases is then obtained. This iterative procedure stops when the new set of the unknowns is close to the previous one.

This method has proved its efficiency and can be found in other more recent works (see for example (4)). However, its quadratic convergence is far from being verified.

3.2 Choice of the integration variables

The integration variables are:

- the macroscopic elastic strain $\underline{E}^{\mathrm{el}}$.
- the macroscopic viscoplastic strain $\underline{E}^{\mathrm{vp}}$.
- the average viscoplastic strains $\underline{\varepsilon}^{\mathrm{vp}(k)}$ of every phases.

The macroscopic equivalent plastic strain P is described as an auxiliary state variable, i.e. is computed after the computation of the integration variables.

Treating the macroscopic viscoplastic strain $\underline{E}^{\mathrm{vp}}$ as an integration variable may seem awkward at this stage, as it can obviously also be treated as an auxiliary state variable. The reason for this choice will become clearer in Section 3.4, where the treatment of the macroscopic viscoplastic strain $\underline{E}^{\mathrm{vp}}$ as an integration variable will appear as a key point of the proposed implicit scheme.

3.3 Derivation of the standard implicit scheme

Let $\vec{Y}$ be a column-vector grouping all the variables:

$$\vec{Y} = \left(\underline{E}^{\mathrm{el}} \quad \underline{E}^{\mathrm{vp}} \quad \underline{\varepsilon}^{\mathrm{vp}(0)} \quad \dots \quad \underline{\varepsilon}^{\mathrm{vp}(N_g)} \right)^T$$

Combining Equations (1), (3), (4) and (5), the evolution of $\vec{Y}$ can be expressed as an ordinary system of differential equations:

$$\dot{\vec{Y}} = G\left(\vec{Y}\right)$$

For a given time step Δt, an implicit scheme consists in replacing this ordinary system of differential equations by a system of non linear equations which unknowns are the increments of the integration variables, as follows:

$$\vec{F}\left(\Delta\vec{Y}\right) = \vec{0} \tag{7}$$

where the residual function $\vec{F}$ is given by:

$$\vec{F}\left(\Delta\vec{Y}\right) = \Delta\vec{Y} - G\left(\vec{Y}\Big|_{t+\theta\Delta t}\right)\Delta t$$

In the previous equation, θ is a numerical parameter ($\theta \in [0,1]$) and the notation $\vec{Y}\Big|_{t+\theta\Delta t}$ denotes:

$$\vec{Y}\Big|_{t+\theta\Delta t} = \vec{Y}\Big|_{t} + \theta\Delta\vec{Y}$$

The unknowns of the implicit system are thus the increment of integration variables:

$$\Delta\underline{E}^{\mathrm{el}}, \Delta\underline{E}^{\mathrm{vp}}, \Delta\underline{\varepsilon}^{\mathrm{vp}(k)}$$

In the following, the residual function $\vec{F}$ is decomposed as follows:

$$\vec{F} = \begin{pmatrix} f_{\underline{E}^{\mathrm{el}}} & f_{\underline{E}^{\mathrm{vp}}} & f_{\underline{\varepsilon}^{\mathrm{vp}(0)}} & \cdots & f_{\underline{\varepsilon}^{\mathrm{vp}(N_g)}} \end{pmatrix}^T$$

The residuals of the implicit systems are given by:

$$\begin{cases} f_{\underline{E}^{\mathrm{el}}} = \Delta\underline{E}^{\mathrm{el}} + \Delta\underline{E}^{\mathrm{vp}} - \Delta\underline{E}^{\mathrm{to}} \\ f_{\underline{E}^{\mathrm{vp}}} = \Delta\underline{E}^{\mathrm{vp}} - \displaystyle\sum_{k=1}^{N_g} \phi^{(k)}\,\Delta\underline{\varepsilon}^{\mathrm{vp}(k)} \\ f_{\underline{\varepsilon}^{\mathrm{vp}(k)}} = \Delta\underline{\varepsilon}^{\mathrm{vp}(k)} - \Delta t\, v^{(k)}\left(\underline{\sigma}^{(k)}\Big|_{t+\theta\Delta t}\right) \end{cases}$$

The residual system (7) is generally solved by a standard Newton-Raphson method which requires the computation of the jacobian matrix $J = \dfrac{\partial F}{\partial \Delta Y}$ which can also be decomposed by blocks.

Due to the expression of $\underline{\sigma}^{(k)}\Big|_{t+\theta\Delta t}$ given by Equation (4), the only not zero jacobian blocks associated with $f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}$ are: $\dfrac{\partial f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}}{\partial \Delta\underline{\varepsilon}^{\mathrm{vp}(k)}}$, $\dfrac{\partial f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}}{\partial \Delta\underline{E}^{\mathrm{el}}}$ and $\dfrac{\partial f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}}{\partial \Delta\underline{\varepsilon}^{\mathrm{vp}}}$. In particular, $\dfrac{\partial f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}}{\partial \Delta\underline{\varepsilon}^{\mathrm{vp}(l)}}$ is null if l is not equal to k.

In the simple case of the simple flow rule described in Equation (5), the expression of those derivatives are:

$$\begin{cases} \dfrac{\partial f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}}{\partial \Delta\underline{\varepsilon}^{\mathrm{vp}(k)}} = \underline{\underline{\mathbf{I}}} - \Delta t \dfrac{\partial v^{(k)}}{\partial \underline{\sigma}^{(k)}} : \dfrac{\partial \underline{\sigma}^{(k)}}{\partial \Delta\underline{\varepsilon}^{\mathrm{vp}(k)}} \\ \dfrac{\partial f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}}{\partial \Delta\underline{E}^{\mathrm{el}}} = -\Delta t \dfrac{\partial v^{(k)}}{\partial \underline{\sigma}^{(k)}} : \dfrac{\partial \underline{\sigma}^{(k)}}{\partial \Delta\underline{E}^{\mathrm{el}}} \\ \dfrac{\partial f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}}{\partial \Delta\underline{E}^{\mathrm{vp}}} = -\Delta t \dfrac{\partial v^{(k)}}{\partial \underline{\sigma}^{(k)}} : \dfrac{\partial \underline{\sigma}^{(k)}}{\partial \Delta\,\underline{E}^{\mathrm{vp}}} \end{cases}$$

Those expressions show that the jacobian block $\dfrac{\partial f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}}{\partial \Delta \underline{\varepsilon}^{\mathrm{vp}(k)}}$ is always invertible for sufficiently small time steps.

At this stage, it must be emphasised that a direct application of this standard Newton-Raphson method would lead to a huge jacobian matrix which would be inefficient in practice, or even untractable for a high number of grains. Hence, the next paragraph is dedicated to a modification of this standard Newton-Raphson scheme which overcomes this issue.

3.4 Static condensation

The Newton correction $\delta \Delta \underline{\varepsilon}^{\mathrm{vp}(k)}$ to the increment of the current estimate of viscoplastic strain increment $\Delta \underline{\varepsilon}^{\mathrm{vp}(k)}$ satisfies:

$$\frac{\partial f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}}{\partial \Delta \underline{\varepsilon}^{\mathrm{vp}(k)}} : \delta \Delta \underline{\varepsilon}^{\mathrm{vp}(k)} + \frac{\partial f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}}{\partial \Delta \underline{E}^{\mathrm{el}}} : \delta \Delta \underline{E}^{\mathrm{el}} + \frac{\partial f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}}{\partial \Delta \underline{E}^{\mathrm{vp}}} : \delta \Delta \underline{E}^{\mathrm{vp}} = -f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}$$

Hence, the Newton correction $\delta \Delta \underline{\varepsilon}^{\mathrm{vp}(k)}$ can be expressed as:

$$\delta \Delta \underline{\varepsilon}^{\mathrm{vp}(k)} = -\left(\frac{\partial f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}}{\partial \Delta \underline{\varepsilon}^{\mathrm{vp}(k)}}\right)^{-1} : \left(\frac{\partial f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}}{\partial \Delta \underline{E}^{\mathrm{el}}} : \delta \Delta \underline{E}^{\mathrm{el}} + \frac{\partial f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}}{\partial \Delta \underline{E}^{\mathrm{vp}}} : \delta \Delta \underline{E}^{\mathrm{vp}} + f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}\right) \tag{8}$$

To simplify the notations, let us introduce the following fourth-order tensors:

$$\underline{\underline{\mathbf{A}}}^{(k)} = \left(\frac{\partial f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}}{\partial \Delta \underline{\varepsilon}^{\mathrm{vp}(k)}}\right)^{-1} : \frac{\partial f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}}{\partial \Delta \underline{E}^{\mathrm{el}}} \quad \text{and} \quad \underline{\underline{\mathbf{B}}}^{(k)} = \left(\frac{\partial f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}}{\partial \Delta \underline{\varepsilon}^{\mathrm{vp}(k)}}\right)^{-1} : \frac{\partial f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}}{\partial \Delta \underline{E}^{\mathrm{vp}}},$$

and the following second-order tensor $\underline{C}^{(k)} = \left(\dfrac{\partial f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}}{\partial \Delta \underline{\varepsilon}^{\mathrm{vp}(k)}}\right)^{-1} : f_{\underline{\varepsilon}^{\mathrm{vp}(k)}}$.

With those tensors, Equation (8) may be rewritten as follows:

$$\delta \Delta \underline{\varepsilon}^{\mathrm{vp}(k)} = -\underline{\underline{\mathbf{A}}}^{(k)} : \delta \Delta \underline{E}^{\mathrm{el}} - \underline{\underline{\mathbf{B}}}^{(k)} : \delta \Delta \underline{E}^{\mathrm{vp}} - \underline{C}^{(k)} \tag{9}$$

Equation (9) can be injected in the equation giving the Newton correction of the increment of the macroscopic viscoplastic strain:

$$\delta \Delta \underline{E}^{\mathrm{vp}} - \sum_{k=1}^{N_g} \phi^{(k)} \, \delta \Delta \underline{\varepsilon}^{\mathrm{vp}(k)} = -f_{\underline{E}^{\mathrm{vp}}}$$

$$\left(\underline{\underline{I}} + \sum_{k=1}^{N_g} \phi^{(k)} \, \underline{\underline{\mathbf{B}}}^{(k)}\right) : \delta \Delta \underline{E}^{\mathrm{vp}} + \sum_{k=1}^{N_g} \phi^{(k)} \, \underline{\underline{\mathbf{A}}}^{(k)} : \delta \Delta \underline{E}^{\mathrm{el}} = -f_{\underline{E}^{\mathrm{vp}}} - \sum_{k=1}^{N_g} \phi^{(k)} \, \underline{C}^{(k)}$$

The correction of the increment of the macroscopic variables satisfies the following condensed system:

$$\begin{pmatrix} \underline{\underline{\mathbf{I}}} & \underline{\underline{\mathbf{I}}} \\ \underline{\underline{\mathbf{J}}}^{(c)}_{\underline{E}^{\mathrm{el}}} & \underline{\underline{\mathbf{J}}}^{(c)}_{\underline{E}^{\mathrm{vp}}} \end{pmatrix} \cdot \begin{pmatrix} \delta \Delta \underline{E}^{\mathrm{el}} \\ \delta \Delta \underline{E}^{\mathrm{vp}} \end{pmatrix} = - \begin{pmatrix} f_{\underline{E}^{\mathrm{el}(k)}} \\ f_{\underline{E}^{\mathrm{vp}(k)}} + \sum_{k=1}^{N_g} \phi^{(k)} \, \underline{C}^{(k)} \end{pmatrix} \tag{10}$$

where the following condensed tensors have been introduced:

$$\underline{\underline{\mathbf{J}}}^{(c)}_{\underline{E}^{\mathrm{el}}} = \sum_{k=1}^{N_g} \phi^{(k)} \, \underline{\underline{\mathbf{A}}}^{(k)} \quad \text{and} \quad \underline{\underline{\mathbf{J}}}^{(c)}_{\underline{E}^{\mathrm{vp}}} = \underline{\underline{I}} + \sum_{k=1}^{N_g} \phi^{(k)} \, \underline{\underline{\mathbf{B}}}^{(k)}.$$

Of course, Linear System (10) may be further condensed to make only appear the correction to increment the macroscopic elastic strain.

3.5 Resolution algorithm

Finally, the local resolution algorithm can be summarized as follows:

1. Given an estimation of the $\Delta\underline{E}^{\mathrm{el}}$, $\Delta\underline{E}^{\mathrm{vp}}$
2. If the iteration number if greater than 1, loop over the phases
   a. Update $\Delta\underline{\varepsilon}^{\mathrm{vp}(k)}$ using Equation (9).
3. Compute $f_{\underline{E}^{\mathrm{el}(k)}}$
4. Loop over the phases and:
   a. Compute the local stress $\underline{\sigma}^{(k)}$
   b. Compute $\underline{\underline{\mathbf{A}}}^{(k)}$, $\underline{\underline{\mathbf{B}}}^{(k)}$, $\underline{C}^{(k)}$,
   c. Update $\underline{\underline{\mathbf{J}}}^{(c)}_{\underline{E}^{\mathrm{el}}}$, $\underline{\underline{\mathbf{J}}}^{(c)}_{\underline{E}^{\mathrm{vp}}}$ and $f^{(c)}_{\underline{E}^{\mathrm{vp}(k)}}$
5. Solve Linear System (10).
6. Update $\Delta\underline{E}^{\mathrm{el}}$, $\Delta\underline{E}^{\mathrm{vp}}$
7. Repeat until convergence

3.6 Computation of the consistent tangent operator

As detailled in (6), the consistent tangent operator can be deduced from the 6×6 left upper part of the invert of the condensed jacobian matrix appearing Equation (10).

4 Some numerical results

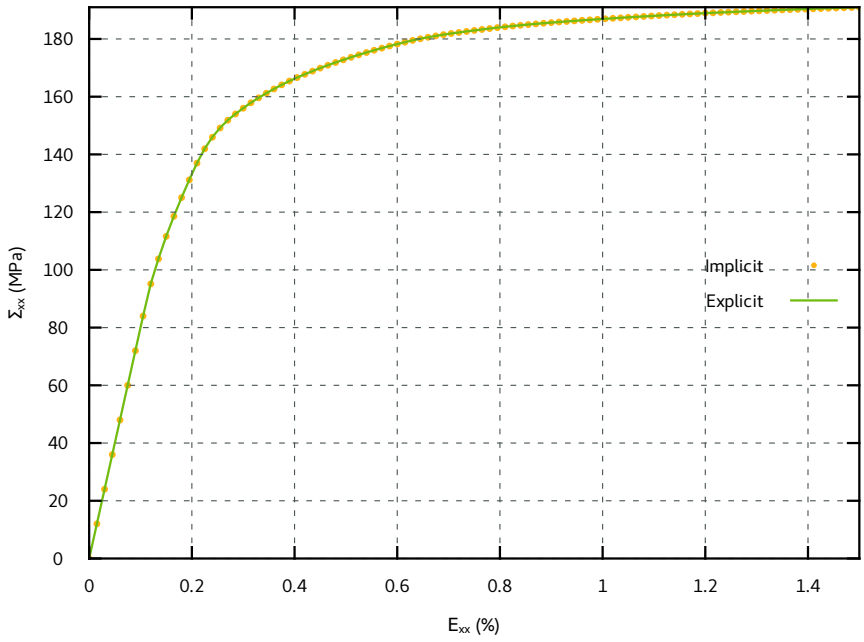

Figure 1: Comparison of the results of the implicit and explicit implementations respectively for a simple uniaxial tensile test

The implicit scheme described in Section 3 has been implemented using the `MFront` code generator (7). An implementation using an explicit integration scheme is also available[2].

Figure 1 compares the results of the implicit and explicit implementations for a simple uniaxial tensile test with an imposed total strain rate using the `MTest` solver delivered with `MFront`, showing very good agreement between the two integration schemes.

[2]The explicit implementation is fully described on this page: https://thelfer.github.io/tfel/web/ExplicitBerveillerZaouiPolyCrystals.html

The local Newton-Raphson appears to converge quadratically which shows that the condensed jacobian matrix appearing in Equation (10) is correctly computed.

The equilibrium equations also exhibit a quadratic convergence showing that the consistent tangent operator is also correctly computed. This has been confirmed by comparing this operation to a numerical approximation.

5 Conclusions

This paper proposed an implicit scheme for polycrystals obtained by a standard homogeneization scheme, which is, to the best of our knowledge original and may be of significant importance for the use of such homogeneized behaviours in structural applications.

This implicit scheme will be extended in a straightforward manner to more complex behaviours and other well-known homogeneization schemes, including Taylor-Lin, Kröner, Cailletaud-Pilvin (β-model), and extensions. Improved self-consistent approaches will also be considered.

The support of complex constitutive laws requires developments in the core of the `MFront` code generator to separate the constitutive equations associated with each phases in a dedicated file and will allow:

- The creation of a dedicated brick[3].
- The parallelisation of the integration of each constitutive equations which may significantly improve the performance of the proposed scheme.

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References

1. Berveiller, M. and Zaoui, A. An extension of the self-consistent scheme to plastically-flowing polycrystals. *Journal of the Mechanics and Physics of Solids*. 1 October 1978. Vol. 26, no. 5, p. 325–344. DOI 10.1016/0022-5096(78)90003-0. Available from: http://www.sciencedirect.com/science/article/pii/0022509678900030

2. Onimus, Fabien and Béchade, Jean-Luc. A polycrystalline modeling of the mechanical behavior of neutron irradiated zirconium alloys. *Journal of Nuclear Materials*. 15 February 2009. Vol. 384, no. 2, p. 163–174. DOI 10.1016/j.jnucmat.2008.11.006. Available from: http://www.sciencedirect.com/science/article/pii/S0022311508006910

3. Hutchinson, John Woodside and Hill, Robert. Bounds and self-consistent estimates for creep of polycrystalline materials. *Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences*. 10 February 1976. Vol. 348, no. 1652, p. 101–127. DOI 10.1098/rspa.1976.0027. Available from: https://royalsocietypublishing.org/doi/10.1098/rspa.1976.0027

4. Bornert, M., Masson, R., Castañeda, P. Ponte and Zaoui, A. Second-order estimates for the effective behaviour of viscoplastic polycrystalline materials. *Journal of the Mechanics and Physics of Solids*. 1 November 2001. Vol. 49, no. 11, p. 2737–2764. DOI 10.1016/S0022-5096(01)00077-1. Available from: http://www.sciencedirect.com/science/article/pii/S0022509601000771

[3] Bricks in `MFront` designates built-in helper features dedicated to a specific class of constitutive equations.

5. Méric, Laurent and Cailletaud, Georges. Single crystal modelling for structural calculations. *Journal of Engineering Material and Technology*. January 1991. Vol. 113, p. 171–182.

6. Helfer, Thomas. Assisted computation of the consistent tangent operator of behaviours integrated using an implicit scheme. Theory and implementation in MFront. Documentation of mfront. CEA, 2020. Available from: https://www.researchgate.net/publication/342721072_Assisted_computation_of_the_consistent_tangent_operator_of_behaviours_integrated_using_an_implicit_scheme_Theory_and_implementation_in_MFront

7. Helfer, Thomas, Michel, Bruno, Proix, Jean-Michel, Salvo, Maxime, Sercombe, Jérôme and Casella, Michel. Introducing the open-source mfront code generator: Application to mechanical behaviours and material knowledge management within the PLEIADES fuel element modelling platform. *Computers & Mathematics with Applications*. September 2015. Vol. 70, no. 5, p. 994–1023. DOI 10.1016/j.camwa.2015.06.027. Available from: http://www.sciencedirect.com/science/article/pii/S0898122115003132