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1 A self-consistent estimate for linear viscoelastic
2 polycrystals with internal variables inferred from the
3 collocation method

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11 **Abstract.** The correspondence principle is customarily used with the Laplace-Carson
12 transform technique to tackle the homogenization of linear viscoelastic heterogeneous
13 media. The main drawback of this method lies in the fact that the whole stress
14 and strain histories have to be considered to compute the mechanical response of the
15 material during a given macroscopic loading. Following a remark of Mandel (1966),
16 Ricaud and Masson (2009) have shown the equivalence between the collocation method
17 used to invert Laplace-Carson transforms and an internal variables formulation. In
18 the present article, this new method is developed for the case of polycrystalline
19 materials with general anisotropic properties for local and macroscopic behaviors.
20 Applications are provided for the case of constitutive relations accounting for glide
21 of dislocations on particular slip systems. It is shown that the method yields accurate
22 results that perfectly match the standard collocation method and reference full-field
23 results obtained with a FFT numerical scheme. The formulation is then extended to
24 the case of time and strain dependent viscous properties, leading to the Incremental
25 Collocation Method (ICM) that can be solved efficiently by a step-by-step procedure.
26 Specifically, the introduction of isotropic and kinematic hardening at the slip system
27 scale is considered.

1. Introduction

The principal issue for the homogenization of linear viscoelastic heterogeneous media is due to memory effects. Owing to the dependence of the local strain-rate on both local stress (viscous response) and stress-rate (elastic response), standard homogenization methods developed for elasticity or viscoplasticity do not apply directly. In particular, the whole stress and strain histories have to be considered for determining the mechanical response at a given time. From the practical point of view of numerical applications, this property requires storing the stress and strain in each mechanical phase for the whole loading path. This can be quite cumbersome especially for polycrystals which are heterogeneous media containing a large number (typically a few thousands) of constituent phases (i.e. crystalline orientations).

Approximate solutions based on properly chosen internal variables have been proposed, e.g. see [1, 2, 3, 4]. Internal variables aim to keep track of the whole stress/strain histories and to summarize their effect on the material behavior. Since their number is limited, the amount of information required to predict the next time step is by far smaller than with hereditary approaches considering full memory effects (at the expense of a lesser accuracy). An alternative internal variable method, based on an incremental variational principle, has been proposed by [5, 6]. By contrast with previous approaches, this method makes use of the recent developments for the homogenization of nonlinear composites which rely on the use of both first and second moments of the mechanical fields to define a linear comparison composite (LCC) [7, 8, 9] and effective internal variables per phase.

The homogenization problem can be solved exactly by making use of the correspondence principle [10]. Taking the Laplace-Carson (LC) transform of the problem, the linear viscoelastic behavior is transformed into a *symbolic* linear elastic one in the LC space. Any linear homogenization model can thus be applied to the fictitious elastic heterogeneous material. Then, inverse LC transforms must be carried out to obtain the viscoelastic effective property in the cartesian space. Except for few simple cases for which this inversion can be performed exactly [11, 12] and besides a simple approximate solution (direct method) which is only accurate for specific loading paths such as creep [13, 14, 15], numerical inversions are generally required. For this goal, approaches relying on Dirichlet series expansion of the original time functions have been proposed, e.g. [13, 16, 17, 18]. Among them, the so-called *collocation method* [13] has provided very good results for the homogenization of polycrystals [19, 20, 21].

Recently, Ricaud and Masson [22] have made use of a remark of [10] showing that an internal variable formulation arises naturally from the collocation method. They illustrated the potentiality of this new method for the case of a two-phase composite with isotropic phases. The main attractive feature of this formulation is to keep the accuracy of integral approaches while preserving the flexibility of an internal variable approach.

The present study develops one step further the approach of Ricaud and Masson

[22]. We consider n -phase polycrystalline materials with general anisotropic properties for local and macroscopic behaviors and applications are provided for constitutive relations accounting for glide of dislocations on particular slip systems. We recall in section 2 the basic equations for the homogenization of thermoviscoelastic heterogeneous media and it is shown in section 3 how internal variables come out naturally from the collocation method, for both stress and strain formulations. Applications are provided for a 2-D isotropic polycrystal submitted to (i) creep loading with stress discontinuities and (ii) complex loading path with strain harmonic loading. In section 4, the method is extended to time- and strain- dependent viscous properties (resulting from isotropic and kinematic hardening on slip systems), which can be solved with a step-by-step procedure. The results obtained for a loading path containing a harmonic part are compared to reference solutions obtained by the FFT full-field numerical approach of [23].

2. Homogenization of linear thermoviscoelastic heterogeneous media

2.1. Constitutive equation for local behavior

According to the Boltzmann superposition principle, the local stress (resp. strain) response of a heterogeneous linear thermoviscoelastic medium can be expressed as a Stieltjes convolution of a viscoelastic stiffness (resp. compliances) tensor with strain (resp. stress), with the addition of thermal stress (resp. strain), that is

$$\begin{aligned}\boldsymbol{\sigma}(\mathbf{x}, t) &= [\mathbf{C} \star \boldsymbol{\varepsilon}](\mathbf{x}, t) + \boldsymbol{\sigma}_0(\mathbf{x}, t) \\ \boldsymbol{\varepsilon}(\mathbf{x}, t) &= [\mathbf{S} \star \boldsymbol{\sigma}](\mathbf{x}, t) + \boldsymbol{\varepsilon}_0(\mathbf{x}, t)\end{aligned}\quad (1)$$

with \mathbf{x} and t the space and time variables, $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ stress and strain tensors, \star the Stieltjes convolution product, \mathbf{C} the viscoelastic stiffness tensor (i.e. relaxation function), and \mathbf{S} the viscoelastic compliance (i.e. creep function). Stieltjes convolutions being defined as the time derivative of Riemann convolutions, the constitutive law is obtained by considering the superimposition of infinitesimal and finite strain increments, $d\boldsymbol{\varepsilon}$ and $d\boldsymbol{\sigma}$,

$$\begin{aligned}\boldsymbol{\sigma}(\mathbf{x}, t) &= \frac{d}{dt} \left[\int_0^t \mathbf{C}(\mathbf{x}, t-u) : \boldsymbol{\varepsilon}(u) du \right] + \boldsymbol{\sigma}_0(\mathbf{x}, t) \\ &= \int_0^t \mathbf{C}(\mathbf{x}, t-u) : \dot{\boldsymbol{\varepsilon}}(u) du + \sum_d \mathbf{C}(\mathbf{x}, t-t_d) : [\boldsymbol{\varepsilon}]_d + \boldsymbol{\sigma}_0(\mathbf{x}, t).\end{aligned}\quad (2)$$

In this expression, strain discontinuities $[\boldsymbol{\varepsilon}]_d$ are considered only for times $t_d < t$. Alternatively, the constitutive behaviour reads

$$\begin{aligned}\boldsymbol{\varepsilon}(\mathbf{x}, t) &= \frac{d}{dt} \left[\int_0^t \mathbf{S}(\mathbf{x}, t-u) : \boldsymbol{\sigma}(u) du \right] + \boldsymbol{\varepsilon}_0(\mathbf{x}, t) \\ &= \int_0^t \mathbf{S}(\mathbf{x}, t-u) : \dot{\boldsymbol{\sigma}}(u) du + \sum_d \mathbf{S}(\mathbf{x}, t-t_d) : [\boldsymbol{\sigma}]_d + \boldsymbol{\varepsilon}_0(\mathbf{x}, t)\end{aligned}\quad (3)$$

with possible stress discontinuities $[\boldsymbol{\sigma}]_d$ at times $t_d < t$.

The creep function of a Maxwell viscoelastic behavior with general anisotropy reads

$$\mathbf{S}(\mathbf{x}, t) = \mathbf{S}^e(\mathbf{x}) + \mathbf{S}^v(\mathbf{x}) t \quad (4)$$

with \mathbf{S}^e and \mathbf{S}^v the elastic and viscous compliances tensors. By definition, the relaxation function $\mathbf{C}(\mathbf{x}, t)$ obeys $\mathbf{C} \star \mathbf{S} = \mathbf{I}$ (\mathbf{I} is the identity tensor) but, unlike the creep function, its analytical expression depends on the class of symmetry (Appendix A).

2.2. Effective behaviour

We consider the case of a polycrystal made of R mechanical phases (i.e. R crystalline orientations) with χ_r the characteristic function of phase r and c_r its volume fraction. The local thermoviscoelastic behavior is maxwellian and uniform in each phase, so that tensors \mathbf{C}^e , \mathbf{C}^v , \mathbf{S}^e , \mathbf{S}^v , \mathbf{C} , \mathbf{S} , $\boldsymbol{\sigma}_0$, $\boldsymbol{\varepsilon}_0$ are also uniform per phase, and denoted \mathbf{C}_r^e , \mathbf{C}_r^v , \mathbf{S}_r^e , \mathbf{S}_r^v , \mathbf{C}_r , \mathbf{S}_r , $\boldsymbol{\sigma}_{0r}$, and $\boldsymbol{\varepsilon}_{0r}(t)$. Thus

$$\begin{aligned} \mathbf{C}(\mathbf{x}, t) &= \sum_r \chi_r(\mathbf{x}) \mathbf{C}_r(t), & \boldsymbol{\sigma}_0(\mathbf{x}, t) &= \sum_r \chi_r(\mathbf{x}) \boldsymbol{\sigma}_{0r}(t) \\ \mathbf{S}(\mathbf{x}, t) &= \sum_r \chi_r(\mathbf{x}) \mathbf{S}_r(t), & \boldsymbol{\varepsilon}_0(\mathbf{x}, t) &= \sum_r \chi_r(\mathbf{x}) \boldsymbol{\varepsilon}_{0r}(t) \end{aligned} \quad (5)$$

with $\mathbf{S}_r(t) = \mathbf{S}_r^e + \mathbf{S}_r^v t$ and $\mathbf{C}_r \star \mathbf{S}_r = \mathbf{I}$. The average stress and strain (denoted $\langle . \rangle_r$) within phase r obey the constitutive relation (1)

$$\begin{aligned} \langle \boldsymbol{\sigma} \rangle_r(t) &= [\mathbf{C}_r \star \langle \boldsymbol{\varepsilon} \rangle_r](t) + \boldsymbol{\sigma}_{0r}(t) \\ \langle \boldsymbol{\varepsilon} \rangle_r(t) &= [\mathbf{S}_r \star \langle \boldsymbol{\sigma} \rangle_r](t) + \boldsymbol{\varepsilon}_{0r}(t) \end{aligned} \quad (6)$$

These phase average fields are linked to macroscopic ones by phase average stress and strain localization tensors $\mathbf{B}_r(t)$ and $\mathbf{A}_r(t)$ ‡

$$\begin{aligned} \langle \boldsymbol{\sigma} \rangle_r(t) &= [\mathbf{B}_r \star \bar{\boldsymbol{\sigma}}](t) + \langle \boldsymbol{\sigma}_{\text{res}} \rangle_r(t) \\ \langle \boldsymbol{\varepsilon} \rangle_r(t) &= [\mathbf{A}_r \star \bar{\boldsymbol{\varepsilon}}](t) + \langle \boldsymbol{\varepsilon}_{\text{res}} \rangle_r(t) \end{aligned} \quad (7)$$

with $\bar{\boldsymbol{\sigma}}$ and $\bar{\boldsymbol{\varepsilon}}$ the overall (macroscopic) stress and strain ($\bar{\boldsymbol{\sigma}} = \langle \boldsymbol{\sigma} \rangle$, $\bar{\boldsymbol{\varepsilon}} = \langle \boldsymbol{\varepsilon} \rangle$, with $\langle . \rangle$ the average over the polycrystal volume). In (7), $\langle \boldsymbol{\varepsilon}_{\text{res}} \rangle_r$ and $\langle \boldsymbol{\sigma}_{\text{res}} \rangle_r$ are the phase average residual stress and strain defined by

$$\begin{aligned} \langle \boldsymbol{\sigma}_{\text{res}} \rangle_r(t) &= [\mathbf{D}_r(t) \star (\tilde{\boldsymbol{\varepsilon}}_0 - \boldsymbol{\varepsilon}_{0r})](t) \\ \langle \boldsymbol{\varepsilon}_{\text{res}} \rangle_r(t) &= [\mathbf{E}_r(t) \star (\tilde{\boldsymbol{\sigma}}_0 - \boldsymbol{\sigma}_{0r})](t) \end{aligned} \quad (8)$$

where $\mathbf{D}_r(t)$ and $\mathbf{E}_r(t)$ are respectively eigenstrain and eigenstress average influence tensors. The macroscopic behavior is given by the effective (denoted $\tilde{.}$) relaxation function, creep function, thermal stress, and stress-free strain, given by

$$\begin{aligned} \tilde{\mathbf{C}}(t) &= \langle \mathbf{C}_r \star \mathbf{A}_r \rangle(t), & \tilde{\boldsymbol{\sigma}}_0(t) &= \langle {}^T \mathbf{A}_r \star \boldsymbol{\sigma}_{0r} \rangle(t), \\ \tilde{\mathbf{S}}(t) &= \langle \mathbf{S}_r \star \mathbf{B}_r \rangle(t), & \tilde{\boldsymbol{\varepsilon}}_0(t) &= \langle {}^T \mathbf{B}_r \star \boldsymbol{\varepsilon}_{0r} \rangle(t). \end{aligned} \quad (9)$$

This homogenization problem can be solved by making use of the correspondence principle [10]. Taking the LC transforms of previous equations, Stieljes convolution

‡ Note that \mathbf{A} and \mathbf{B} are not necessarily uniform per phase

120 products are transformed into simple scalar products, and therefore the original
 121 thermoviscoelastic homogenization problem is transformed into a *symbolic* thermoelastic
 122 homogenization problem for which standard homogenization techniques apply. Let f^*
 123 denotes the LC transform of function f , $f^*(p) = p \int_0^\infty f(t)e^{-pt}dt$ with p the complex
 124 variable. The symbolic thermoelastic behavior thus reads

$$\begin{aligned} \tilde{\mathbf{C}}^*(p) &= \langle \mathbf{C}_r^*(p) : \mathbf{A}_r^*(p) \rangle, & \tilde{\boldsymbol{\sigma}}_0^*(p) &= \langle {}^T \mathbf{A}_r^*(p) : \boldsymbol{\sigma}_{0r}^*(p) \rangle \\ \tilde{\mathbf{S}}^*(p) &= \langle \mathbf{S}_r^*(p) : \mathbf{B}_r^*(p) \rangle, & \tilde{\boldsymbol{\varepsilon}}_0^*(p) &= \langle {}^T \mathbf{B}_r^*(p) : \boldsymbol{\varepsilon}_{0r}^*(p) \rangle \end{aligned} \quad (10)$$

125 with \mathbf{S}_r^* , \mathbf{C}_r^* , $\boldsymbol{\varepsilon}_{0r}^*$ and $\boldsymbol{\sigma}_{0r}^*$ symbolic thermoelastic property tensors. Once the
 126 homogenization problem has been solved in the LC space, the solution has to be
 127 inverse transformed back to the original time space. This inversion constitutes the
 128 main difficulty for thermoviscoelastic homogenization. In this work, use will be made of
 129 the collocation method [13]. Following [22], it will be shown that an internal variables
 130 formulation can be naturally derived from this inversion procedure, without additional
 131 assumptions. It is also pointed out that this feature is not restricted to this specific
 132 numerical inversion method.

133 3. A formulation based on internal variables inferred from the collocation 134 method

135 3.1. The collocation method

136 It is assumed that the considered polycrystal is subjected to a given derivable stress
 137 loading path $\bar{\boldsymbol{\sigma}}(u)$, $u \in [0; t]$ with additional discontinuities (i.e. stress jumps) $[\bar{\boldsymbol{\sigma}}]_d$ at
 138 times t_d , and initial conditions $\boldsymbol{\sigma}(\mathbf{x}, 0) = \bar{\boldsymbol{\sigma}}(0) = \mathbf{0} \forall(\mathbf{x})$. The overall polycrystal
 139 response $\bar{\boldsymbol{\varepsilon}}(t)$ reads

$$140 \quad \bar{\boldsymbol{\varepsilon}}(t) = \int_0^t \tilde{\mathbf{S}}(t-u) : \dot{\bar{\boldsymbol{\sigma}}}(u) du + \sum_d \tilde{\mathbf{S}}(t-t_d) : [\bar{\boldsymbol{\sigma}}]_d + \tilde{\boldsymbol{\varepsilon}}_0(t). \quad (11)$$

141 The collocation method is based on an approximation of the effective creep function $\tilde{\mathbf{S}}$
 142 by a Dirichlet serie $\tilde{\mathbf{S}}^{ap}$

$$143 \quad \tilde{\mathbf{S}}(t) \approx \tilde{\mathbf{S}}^{ap}(t) = \tilde{\mathbf{S}}^e + \tilde{\mathbf{S}}^v t + \sum_{s=1}^{S_c} \mathbf{S}_{\tau_s} (1 - e^{-\frac{t}{\tau_s}}) \quad (12)$$

144 which LC transform reads

$$145 \quad \tilde{\mathbf{S}}^{ap*}(p) = \tilde{\mathbf{S}}^e + \frac{1}{p} \tilde{\mathbf{S}}^v + \sum_{s=1}^{S_c} \mathbf{S}_{\tau_s} \frac{1}{1 + \tau_s p}. \quad (13)$$

146 The S_c collocation times τ_s can be chosen optimally as in [24], but here they are supposed
 147 to be determined *a priori*. Equation (13) defines a system of S_c linear equations, in
 148 which the S_c unknown tensors \mathbf{S}_{τ_s} are determined from the purely elastic and purely
 149 viscous end member solutions (that can be solved independently), and from the symbolic
 150 response $\tilde{\mathbf{S}}^{ap*}(p)$ computed at S_c collocation times $p = 1/\tau_s$. The effective strain response
 151 can then be obtained analytically with relation (11) for any loading path. This method
 152 has been used for polycrystalline materials e.g. in [19, 20, 21].

153 3.2. Stress formulation

154 Alternatively, the macroscopic strain can be obtained by substituting $\tilde{\mathbf{S}}(t)$ in (11) by
 155 its approximation $\tilde{\mathbf{S}}^{ap}(t)$. Integrating by part and using condition $\bar{\boldsymbol{\varepsilon}}(0) = \mathbf{0}$ leads to

$$\begin{aligned} \bar{\boldsymbol{\varepsilon}}(t) = \tilde{\mathbf{S}}^e : \left(\bar{\boldsymbol{\sigma}}(t) + \sum_d [\bar{\boldsymbol{\sigma}}]_d \right) + \tilde{\mathbf{S}}^v : \left(\boldsymbol{\xi}(t) + \sum_d (t - t_d) [\bar{\boldsymbol{\sigma}}]_d \right) + \\ \sum_{s=1}^{S_c} \mathbf{S}_{\tau_s} : \left(\boldsymbol{\beta}_{\tau_s}(t) + \sum_d (1 - e^{-\frac{-(t-t_d)}{\tau_s}}) [\bar{\boldsymbol{\sigma}}]_d \right) + \tilde{\boldsymbol{\varepsilon}}_0(t) \end{aligned} \quad (14)$$

156 where two tensorial internal variables $\boldsymbol{\xi}(t)$ and $\boldsymbol{\beta}_{\tau_s}(t)$ arise naturally. They only depend
 157 on the macroscopic stress path

$$\boldsymbol{\beta}_{\tau_s}(t) = \frac{1}{\tau_s} e^{-\frac{t}{\tau_s}} \int_0^t e^{\frac{u}{\tau_s}} \bar{\boldsymbol{\sigma}}(u) du, \quad \boldsymbol{\xi}(t) = \int_0^t \bar{\boldsymbol{\sigma}}(u) du, \quad (15)$$

159 and are solution of the following differential equations

$$\dot{\boldsymbol{\beta}}_{\tau_s}(t) + \frac{1}{\tau_s} \boldsymbol{\beta}_{\tau_s}(t) = \frac{1}{\tau_s} \bar{\boldsymbol{\sigma}}(t), \quad \dot{\boldsymbol{\xi}}(t) = \bar{\boldsymbol{\sigma}}(t) \quad (16)$$

161 with $\boldsymbol{\beta}_{\tau_s}(0) = \mathbf{0}$, $\boldsymbol{\xi}(0) = \mathbf{0}$. Therefore $\boldsymbol{\xi}$ and $\boldsymbol{\beta}_{\tau_s}$ are macroscopic variables. Remark that
 162 there is a single $\boldsymbol{\xi}$ but as many $\boldsymbol{\beta}_{\tau_s}$ as collocation times. It is also worth noting that
 163 equations (14-16) could be written alternatively by incorporating stress discontinuities
 164 $[\bar{\boldsymbol{\sigma}}]_d$ into the definitions of $\boldsymbol{\xi}$ and $\boldsymbol{\beta}_{\tau_s}$. If the overall polycrystal loading is performed in
 165 such a way that $\bar{\boldsymbol{\varepsilon}}(t)$ is prescribed and $\bar{\boldsymbol{\sigma}}(t)$ is the wanted response, then $\bar{\boldsymbol{\sigma}}(t)$ can
 166 be replaced in the above equations (16) by its expression derived from (14). The
 167 effective thermal strain $\tilde{\boldsymbol{\varepsilon}}_0(t)$ can be expressed by approximating the phase average
 168 stress concentration tensors by a Dirichlet serie, as in [21]

$$\mathbf{B}_r(t) \approx \mathbf{B}_r^{ap}(t) = \mathbf{B}_r^v + \sum_{s=1}^{S_c} \mathbf{B}_{r\tau_s} e^{-\frac{t}{\tau_s}} \quad (17)$$

170 leading to

$$\mathbf{B}_r^{ap*}(p) = \mathbf{B}_r^v + \sum_{s=1}^{S_c} \mathbf{B}_{r\tau_s} \frac{\tau_s p}{1 + \tau_s p} \quad (18)$$

172 where \mathbf{B}_r^v denotes stress concentration tensors for the purely viscous behavior. Tensors
 173 $\mathbf{B}_{r\tau_s}$ can be easily determined from the knowledge of \mathbf{B}_r^{ap*} at collocation times $p = 1/\tau_s$,
 174 and satisfy $\mathbf{B}_r^v + \sum_{s=1}^Q \mathbf{B}_{r\tau_s} = \mathbf{B}_r^e$ with \mathbf{B}_r^e the stress concentration tensor for the purely
 175 elastic behavior. Using this approximation with the initial condition $\boldsymbol{\varepsilon}_{0r}(0) = \mathbf{0}$, relation
 176 (9d) becomes

$$\begin{aligned} \tilde{\boldsymbol{\varepsilon}}_0(t) = \left\langle {}^T \mathbf{B}_r^e : \boldsymbol{\varepsilon}_{0r}(t) + {}^T \mathbf{B}_r^v : \sum_d [\boldsymbol{\varepsilon}_{0r}]_d \right\rangle + \\ \left\langle \sum_s {}^T \mathbf{B}_{r\tau_s} : \left(\sum_d e^{-\frac{-(t-t_d)}{\tau_s}} [\boldsymbol{\varepsilon}_{0r}]_d - \boldsymbol{\eta}_{r\tau_s}(t) \right) \right\rangle \end{aligned} \quad (19)$$

177 with the new internal variable $\boldsymbol{\eta}_{r\tau_s}$ depending only on the thermal stress-free strain and
 178 satisfying

$$179 \quad \dot{\boldsymbol{\eta}}_{r\tau_s}(t) + \frac{1}{\tau_s} \boldsymbol{\eta}_{r\tau_s}(t) = \frac{1}{\tau_s} \boldsymbol{\varepsilon}_{0r}(t), \quad \boldsymbol{\eta}_{r\tau_s}(0) = \mathbf{0}. \quad (20)$$

180 Hence, $\boldsymbol{\eta}_{r\tau_s}$ is a local variable, and it is worth noting that it is homogeneous per phase
 181 due to the homogeneity of $\boldsymbol{\varepsilon}_{0r}$. It is stressed that the three internal variables determined
 182 so far, namely $\boldsymbol{\xi}$, $\boldsymbol{\beta}_{\tau_s}$, and $\boldsymbol{\eta}_{r\tau_s}$, can be calculated in advance as far as the macroscopic
 183 stress and thermal loadings are known and provided the necessary collocation times τ_s
 184 have been fixed. An important consequence of these developments is that the integral
 185 expression (11) for the thermoviscoelastic effective behavior has been replaced by the
 186 internal variable formulation given by (14) and (19) that can be advantageously solved
 187 by means of an incremental numerical procedure.

188 Similarly, the phase average stress defined by the integral equation (7) can be
 189 expressed with respect to internal variables, using the approximation (17) and assuming
 190 a similar form for the eigenstrain influence tensors $\mathbf{D}_r(t)$

$$191 \quad \mathbf{D}_r(t) \approx \mathbf{D}_r^{ap}(t) = \mathbf{D}_r^v + \sum_{s=1}^{S_c} \mathbf{D}_{r\tau_s} e^{-\frac{t}{\tau_s}}. \quad (21)$$

192 This leads to

$$\langle \boldsymbol{\sigma} \rangle_r(t) = \mathbf{B}_r^e : \bar{\boldsymbol{\sigma}}(t) + \mathbf{B}_r^v : \sum_d [\bar{\boldsymbol{\sigma}}]_d + \sum_s \mathbf{B}_{r\tau_s} : \left(\sum_d e^{-\frac{-(t-t_d)}{\tau_s}} [\bar{\boldsymbol{\sigma}}]_d - \boldsymbol{\beta}_{\tau_s}(t) \right) + \langle \boldsymbol{\sigma}_{\text{res}} \rangle_r(t), \quad (22)$$

193

$$\langle \boldsymbol{\sigma}_{\text{res}} \rangle_r(t) = \mathbf{D}_r^e : (\tilde{\boldsymbol{\varepsilon}}_0 - \boldsymbol{\varepsilon}_{0r})(t) + \mathbf{D}_r^v : \sum_d [\tilde{\boldsymbol{\varepsilon}}_0 - \boldsymbol{\varepsilon}_{0r}]_d + \sum_s \mathbf{D}_{r\tau_s} : \left(\sum_d e^{-\frac{-(t-t_d)}{\tau_s}} [\tilde{\boldsymbol{\varepsilon}}_0 - \boldsymbol{\varepsilon}_{0r}]_d - \boldsymbol{\lambda}_{r\tau_s}(t) \right) \quad (23)$$

194 with the new local internal variable $\boldsymbol{\lambda}_{r\tau_s}$ verifying

$$195 \quad \dot{\boldsymbol{\lambda}}_{r\tau_s}(t) + \frac{1}{\tau_s} \boldsymbol{\lambda}_{r\tau_s}(t) = \frac{1}{\tau_s} (\tilde{\boldsymbol{\varepsilon}}_0 - \boldsymbol{\varepsilon}_{0r})(t), \quad \boldsymbol{\lambda}_{r\tau_s}(0) = \mathbf{0}. \quad (24)$$

196 The phase average strain $\langle \boldsymbol{\varepsilon} \rangle_r(t)$ can be eventually computed by solving incrementally
 197 the local constitutive thermoviscoelastic relation.

198 3.3. Strain formulation

199 We now consider that the polycrystal is subjected to a given derivable loading path
 200 $\bar{\boldsymbol{\varepsilon}}(u)$, $u \in [0; t]$ with additional discontinuities $[\bar{\boldsymbol{\varepsilon}}]_d$ at times t_d and initial conditions
 201 $\boldsymbol{\varepsilon}(\mathbf{x}, 0) = \bar{\boldsymbol{\varepsilon}}(0) = \mathbf{0} \forall(\mathbf{x})$. The stress response $\bar{\boldsymbol{\sigma}}(t)$ obtained by the strain (or dual)
 202 formulation reads

$$203 \quad \bar{\boldsymbol{\sigma}}(t) = \int_0^t \tilde{\mathbf{C}}(t-u) : \dot{\bar{\boldsymbol{\varepsilon}}}(u) du + \sum_d \tilde{\mathbf{C}}(t-t_d) : [\bar{\boldsymbol{\varepsilon}}]_d + \tilde{\boldsymbol{\sigma}}_0(t). \quad (25)$$

204 Approximating the effective relaxation function by a Dirichlet series in a form consistent
205 with (12)

$$206 \quad \tilde{\mathbf{C}}(t) \approx \tilde{\mathbf{C}}^{ap}(t) = \sum_{s=1}^{S_c} \mathbf{C}_{\tau_s} e^{-\frac{t}{\tau_s}}, \quad \sum_{s=1}^{S_c} \mathbf{C}_{\tau_s} = \tilde{\mathbf{C}}^e, \quad (26)$$

207 the macroscopic stress reads

$$208 \quad \bar{\boldsymbol{\sigma}}(t) = \tilde{\mathbf{C}}^e : \bar{\boldsymbol{\varepsilon}}(t) - \sum_{s=1}^{S_c} \mathbf{C}_{\tau_s} : \left(\boldsymbol{\alpha}_{\tau_s}(t) - \sum_d e^{-\frac{(t-t_d)}{\tau_s}} [\bar{\boldsymbol{\varepsilon}}]_d \right) + \tilde{\boldsymbol{\sigma}}_0(t) \quad (27)$$

209 with the macroscopic internal variable $\boldsymbol{\alpha}_{\tau_s}$ verifying

$$210 \quad \dot{\boldsymbol{\alpha}}_{\tau_s}(t) + \frac{1}{\tau_s} \boldsymbol{\alpha}_{\tau_s}(t) = \frac{1}{\tau_s} \bar{\boldsymbol{\varepsilon}}(t), \quad \boldsymbol{\alpha}_{\tau_s}(0) = \mathbf{0}. \quad (28)$$

211 The effective thermal stress $\tilde{\boldsymbol{\sigma}}_0(t)$ can be expressed by using the following approximation
212 for the average strain concentration tensors

$$213 \quad \mathbf{A}_r(t) \approx \mathbf{A}_r^{ap}(t) = \mathbf{A}_r^v + \sum_{s=1}^{S_c} \mathbf{A}_{r\tau_s} e^{-\frac{t}{\tau_s}} \quad (29)$$

214 where \mathbf{A}_r^v denotes the strain concentration tensors for the purely viscous behavior.
215 Tensors $\mathbf{A}_{r\tau_s}$ satisfy $\mathbf{A}_r^v + \sum_{s=1}^Q \mathbf{A}_{r\tau_s} = \mathbf{A}_r^e$ with \mathbf{A}_r^e the average strain concentration
216 tensor for the purely elastic behavior. Relation (9b) thus gives

$$\begin{aligned} \tilde{\boldsymbol{\sigma}}_0(t) = & \left\langle {}^T \mathbf{A}_r^e : \boldsymbol{\sigma}_{0r}(t) + {}^T \mathbf{A}_r^v : \sum_d [\boldsymbol{\sigma}_{0r}]_d \right\rangle + \\ & \left\langle \sum_s {}^T \mathbf{A}_{r\tau_s} : \left(\sum_d e^{-\frac{(t-t_d)}{\tau_s}} [\boldsymbol{\sigma}_{0r}]_d - \boldsymbol{\varrho}_{r\tau_s}(t) \right) \right\rangle \end{aligned} \quad (30)$$

217 with $\boldsymbol{\varrho}_{r\tau_s}$ the new internal variable verifying

$$218 \quad \dot{\boldsymbol{\varrho}}_{r\tau_s}(t) + \frac{1}{\tau_s} \boldsymbol{\varrho}_{r\tau_s}(t) = \frac{1}{\tau_s} \boldsymbol{\sigma}_{0r}(t), \quad \boldsymbol{\varrho}_{r\tau_s}(0) = \mathbf{0}. \quad (31)$$

219 As for the stress formulation, the integral expression (25) of the thermoviscoelastic
220 constitutive relation has been replaced by an internal variables approach defined by
221 relations (27) and (30).

222 Detailed equations for the phase average strain are not given here for the sake of
223 conciseness, but they can be obtained using similar developments as those presented
224 above for the stress formulation. Approximating $\mathbf{E}_r(t)$ by a Dirichlet series as $\mathbf{D}_r(t)$,
225 see equation (21), the expressions obtained for $\langle \boldsymbol{\varepsilon} \rangle_r(t)$ and $\langle \boldsymbol{\varepsilon}_{\text{res}} \rangle_r(t)$ have a very similar
226 form to those given above for $\langle \boldsymbol{\sigma} \rangle_r(t)$ and $\langle \boldsymbol{\sigma}_{\text{res}} \rangle_r(t)$.

227 3.4. Application

228 The capabilities of the new formulation with internal variables based on the collocation
229 method are now illustrated for the homogenization problem of a 2-D polycrystal with
230 local anisotropic behavior. Two applications are provided below, the first for prescribed

231 overall stress, and the second for prescribed strain. The model has been implemented
 232 for both stress and strain formulations in order to compare the relative merit and ease of
 233 the numerical implementations. Results will be also compared to the original collocation
 234 method.

235 The chosen microstructure consists of two ($R = 2$) randomly mixed phases, and
 236 it is deformed under antiplane shear. The choice of such a simple microstructure aims
 237 to obtain a rapid validation of the method, but it is not a limitation. The viscoplastic
 238 behavior of similar microstructures has been investigated e.g. in [25, 26, 27]. Owing to
 239 this particular microstructure, the Self-Consistent (SC) scheme has been chosen here to
 240 solve the symbolic linear thermo-elastic homogenization problem in the LC space. Local
 241 elastic and viscous compliances are given by

$$\mathbf{S}_r^e = \sum_{k=1}^2 \frac{1}{4\mu^{e(k)}} \mathbf{R}_r^{(k)} \otimes \mathbf{R}_r^{(k)}, \quad \mathbf{S}_r^v = \sum_{k=1}^2 \frac{1}{\mu^{v(k)}} \mathbf{R}_r^{(k)} \otimes \mathbf{R}_r^{(k)} \quad (32)$$

242 with $\mu^{e(k)}$ and $\mu^{v(k)}$ the elastic and viscous shear compliances of slip system (k).
 243 The following values have been considered for the computations: $\mu^{e(1)} = 1\text{MPa}$,
 244 $\mu^{v(1)} = 2\text{MPa.s}$, $\mu^{e(2)} = 100\text{MPa}$, $\mu^{v(2)} = 20\text{MPa.s}$, so that system (2) is stiff compared
 245 to system (1). The two mechanical phases are rotated by 90° from each other, and
 246 slip is allowed on two perpendicular slip planes along direction \mathbf{e}_3 so that the Schmid
 247 tensors read $\mathbf{R}_2^{(k)} = \frac{1}{2}(\mathbf{e}_k \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_k)$, $\mathbf{R}_1^{(1)} = \mathbf{R}_2^{(2)}$, and $\mathbf{R}_1^{(2)} = -\mathbf{R}_2^{(1)}$ (see figure
 248 3). From the numerical point of view, differential equations appearing in the internal
 249 variables formulation have been solved by the Runge-Kutta method. Collocation times
 250 τ_s have been distributed on a logarithmic scale between the two extreme relaxation
 251 times $\mu^{v(2)}/\mu^{e(2)}$ and $\mu^{v(1)}/\mu^{e(1)}$; numerical applications have been performed for different
 252 numbers of collocation times, $5 \leq S_c \leq 20$, with no influence on results.

253 Several macroscopic loadings have been tested. The first case of interest is a creep
 254 test $\bar{\sigma}_{13}$ including a stress jump

$$\begin{cases} \bar{\sigma}_{13} = 1\text{MPa} & \text{for } t \leq 2\text{s} \\ \bar{\sigma}_{13} = 4\text{MPa} & \text{for } t > 2\text{s} \end{cases} \quad (33)$$

256 The predicted macroscopic behavior, phase average stress, and phase average strain, are
 257 shown in figure 1. These results have been obtained by means of the original collocation
 258 method and the new stress (§3.2) and strain (§3.3) formulations. They are all plotted
 259 in figure 1. It can be seen that results obtained with those three formulations are in
 260 perfect match with each other at both macroscopic and local levels, which validates
 261 the numerical resolution of present developments. It is worth recalling that those three
 262 formulation are equivalent, as discussed above. In particular, the stress jumps at $t = 0\text{s}$
 263 and $t = 2\text{s}$ and subsequent recovery of both phases are nicely captured.

264 Another example of challenging test is the response under harmonic loading. We
 265 have studied the case of a strain imposed antiplane shear with a constant strain-rate

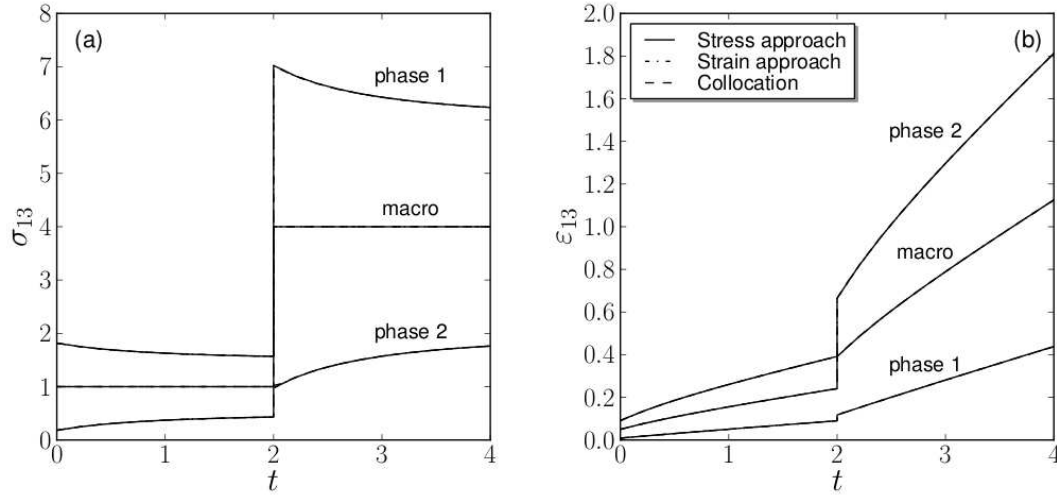


Figure 1. Response of the 2-D polycrystal under the creep loading with stress jump (33). (a) Stress response: ‘macro’ indicates the prescribed $\bar{\sigma}_{13}(t)$, ‘phase 1’ indicates $\langle \sigma_{13} \rangle_1(t)$, and ‘phase 2’ $\langle \sigma_{13} \rangle_2(t)$. (b) Corresponding strain response ($\bar{\epsilon}_{13}(t)$, $\langle \epsilon_{13} \rangle_1(t)$, and $\langle \epsilon_{13} \rangle_2(t)$). Results from the original collocation method and for both stress and strain approaches are shown.

266 stage followed by a sinusoidal overall strain stage, as in [5]

$$267 \quad \begin{cases} \bar{\epsilon}_{13} = A\omega t & \text{for } t \leq t_0 \\ \bar{\epsilon}_{13} = A \sin[\omega(t - t_0)] & \text{for } t > t_0 \end{cases} \quad (34)$$

268 with numerical values $A = 0.04$, $\omega = 15\text{s}^{-1}$, and $t_0 = 1\text{s}$. As for the previous
 269 example, it is found that the three approaches, namely standard collocation method,
 270 stress formulation, and strain formulation provide the same results (figure 2), for the
 271 macroscopic behavior but also for phase average stress and strain. At large time, the
 272 overall specimen has relaxed from the first loading stage and therefore macroscopic stress
 273 and phase average stresses tend to periodic oscillations around 0MPa.

274 To check the validity of these results, reference solutions were generated with a
 275 full-field numerical approach based on Fourier Transforms. The method is described in
 276 [23, 28] for elastic or viscoplastic composites and polycrystals, and in [29] (with numerical
 277 details in [30]) for elasto-viscoplastic behavior. The FFT-based full-field formulation
 278 is conceived for periodic unit cells deformed under periodic boundary conditions, and
 279 it provides the “exact” (within numerical accuracy) solution of the governing equations.
 280 Here, we considered a periodic tile microstructure formed by square grains (see figure
 281 3) which has been found to provide numerical results in very good agreement with
 282 theoretical solutions [31] (with which the linear SC scheme also coincides). For linear
 283 viscoelastic behaviors, the relaxation spectra of this microstructure exhibits an infinite
 284 number of relaxation times. With macroscopic loading (34), the detailed distribution
 285 of stress and strain is thus obtained. For the purpose of comparison with mean-field
 286 homogenization models, stress and strain fields have been spatially averaged to evaluate

287 phase average quantities. Comparison is provided in figure 2. It turns out that results
 288 from the internal variable approaches are virtually undistinguishable from FFT ones,
 289 which proves the accuracy of the proposed method for anisotropic linear viscoelastic
 290 behavior although the method only accounts for a finite (and small) number of relaxation
 291 times.

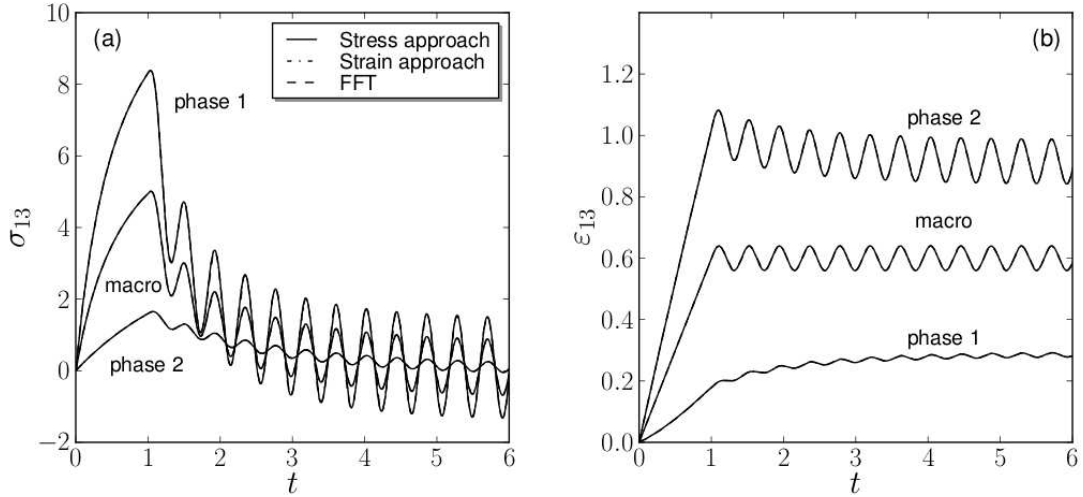


Figure 2. Response of the 2-D polycrystal under the harmonic loading given by (34). Macroscopic and phase average (a) stress and (b) strain responses, as in figure 1. Results from the original collocation method and from both stress and strain approaches are shown, together with those obtained by FFT full-field numerical method.

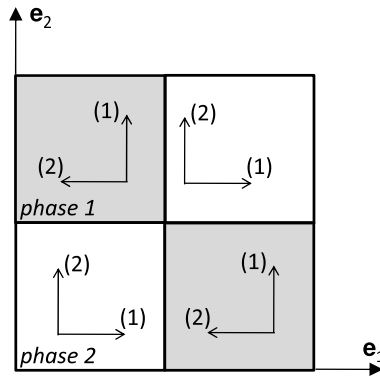


Figure 3. Periodic 2-D microstructure considered for FFT numerical computations. Arrows indicate the normal of slip planes. Slip direction is along \mathbf{e}_3 .

292 4. Extension to time- and strain-dependent viscous properties

293 The above formulation has been provided for constant elastic \mathbf{S}_r^e and viscous \mathbf{S}_r^v
 294 compliances. An important consequence of this feature is that coefficients \mathbf{S}_{τ_s} in (12)

295 have to be determined only once, independently of the macroscopic prescribed loading.
 296 We are now extending the formulation to situations for which this is no more the
 297 case. For illustrative purpose, we are considering the case of local constitutive relations
 298 including isotropic and kinematic hardening, the latter being time-dependent due to
 299 static relaxation mechanisms.

300 4.1. Local constitutive behavior law including hardening and recovery

301 We consider a local constitutive relation (proposed in [30]) with constant elastic
 302 properties, but with a viscous part depending on strain due to isotropic and kinematic
 303 hardening and on time due to static relaxation. We consider Voce-type law for isotropic
 304 hardening and a simple saturating expression for kinematic hardening as in [32]. The
 305 complete constitutive relation reads (spatial position \mathbf{x} has been omitted)

$$\dot{\boldsymbol{\epsilon}} = \mathbf{S}_r^e : \dot{\boldsymbol{\sigma}} + \dot{\boldsymbol{\epsilon}}^v \quad (35)$$

$$\dot{\boldsymbol{\epsilon}}^v = \sum_{k=1}^K \dot{\gamma}^{(k)} \mathbf{R}_r^{(k)} \quad (36)$$

$$\dot{\gamma}^{(k)} = \dot{\gamma}_0 \frac{\tau^{(k)} - X^{(k)}}{\tau_0^{(k)}} \quad (37)$$

$$\tau^{(k)} = \mathbf{R}_r^{(k)} : \boldsymbol{\sigma} \quad (38)$$

$$\dot{\tau}_0^{(k)} = (\tau_{sta}^{(k)} - \tau_0^{(k)}) \sum_{l=1}^K H^{(k,l)} |\dot{\gamma}^{(l)}| \quad (39)$$

$$\dot{X}^{(k)} = c \dot{\gamma}^{(k)} - d X^{(k)} |\dot{\gamma}^{(k)}| - e |X^{(k)}|^m \text{sign}(X^{(k)}) \quad (40)$$

306 with $\dot{\boldsymbol{\epsilon}}^v$ the local viscous strain-rate, $\dot{\gamma}^{(k)}$ the shear-rate on slip system (k), $\tau^{(k)}$ the
 307 resolved shear stress on that system, and $\dot{\gamma}_0$, c , d , and e constant coefficients. With
 308 this law, the reference shear stress $\tau_0^{(k)}$ for system (k) evolves from an initial value to
 309 a saturation value $\tau_{sta}^{(k)}$ due to isotropic hardening, H being the (constant) interaction
 310 matrix between slip systems. Kinematic hardening is due to the backstress $X^{(k)}$ that
 311 includes static recovery (coefficient e). This viscoelastic behavior can be also written

$$\dot{\boldsymbol{\epsilon}} = \mathbf{S}_r^e : \dot{\boldsymbol{\sigma}} + \mathbf{S}^v : \boldsymbol{\sigma} + \dot{\boldsymbol{\epsilon}}_0 \quad (41)$$

313 with

$$\mathbf{S}^v = \sum_{k=1}^K \dot{\gamma}_0^{(k)} \frac{\mathbf{R}_r^{(k)} \otimes \mathbf{R}_r^{(k)}}{\tau_0^{(k)}}, \quad \dot{\boldsymbol{\epsilon}}_0 = - \sum_{k=1}^K \dot{\gamma}_0^{(k)} \frac{X^{(k)} \mathbf{R}_r^{(k)}}{\tau_0^{(k)}}. \quad (42)$$

314 It is worth noting that the above constitutive relation is defined at any point \mathbf{x} within
 315 the polycrystal. Therefore, $\dot{\tau}_0^{(k)}(\mathbf{x})$ and $\dot{X}^{(k)}(\mathbf{x})$ should be heterogeneous within each
 316 mechanical phase due to the intraphase heterogeneity of $\dot{\gamma}^{(k)}(\mathbf{x})$. A consequence of this is
 317 that the compliance $\mathbf{S}^v(\mathbf{x})$ and the stress-free strain $\dot{\boldsymbol{\epsilon}}_0(\mathbf{x})$ are also heterogeneous within
 318 phases, but then standard homogenization techniques do not apply. To circumvent this
 319 difficulty, we have replaced $\dot{\gamma}^{(k)}(\mathbf{x})$ in equations (39) and (40) by its phase average value
 320 $\langle \dot{\gamma}^{(k)} \rangle_r$ so that, starting with phase uniform $\dot{\tau}_0^{(k)}$ and $\dot{X}^{(k)}$ (now denoted $\dot{\tau}_{0r}^{(k)}$ and $\dot{X}_r^{(k)}$),

321 \mathbf{S}^v and $\dot{\boldsymbol{\epsilon}}_0$ remain phase uniform (denoted \mathbf{S}_r^v and $\dot{\boldsymbol{\epsilon}}_{0r}$) so that mean-field homogenization
 322 can be carried out. The phase average behavior thus reads

$$323 \quad \langle \dot{\boldsymbol{\epsilon}} \rangle_r = \mathbf{S}_r^e : \langle \dot{\boldsymbol{\sigma}} \rangle_r + \mathbf{S}_r^v : \langle \boldsymbol{\sigma} \rangle_r + \dot{\boldsymbol{\epsilon}}_{0r} . \quad (43)$$

324 The consequence of this approximation will be discussed below.

325 4.2. The Incremental Collocation Method (ICM)

326 In section 3, both stress and strain approaches have been treated and applied
 327 simultaneously, and we have shown that both provide identical results. In the following,
 328 for the sake of clarity, only the stress formulation is presented (but we have checked that
 329 the strain approach still provides equivalent results) and stress jumps are not included.

330 The main issue comes from the evolution of the viscous local behavior with time and
 331 strain. As a consequence, the coefficients \mathbf{S}_{τ_s} and the homogenized viscous compliance
 332 $\tilde{\mathbf{S}}^v$ evolve so that the homogenization procedure cannot be applied the same way as
 333 previously. This issue can be solved with an *incremental* resolution, assuming that
 334 coefficients \mathbf{S}_{τ_s} are constant during a sufficiently small time increment. Then, equation
 335 (14) becomes

$$336 \quad \Delta \bar{\boldsymbol{\epsilon}} = \tilde{\mathbf{S}}^e : \Delta \bar{\boldsymbol{\sigma}} + \tilde{\mathbf{S}}^v|_{1/2} : \Delta \boldsymbol{\xi} + \sum_{s=1}^S \mathbf{S}_{\tau_s}|_{1/2} : \Delta \boldsymbol{\beta}_{\tau_s} + \Delta \tilde{\boldsymbol{\epsilon}}_0 \quad (44)$$

337 with Δ denoting the increment between times t_n and t_{n+1} , e.g. $\Delta \bar{\boldsymbol{\epsilon}} = \bar{\boldsymbol{\epsilon}}(t_{n+1}) - \bar{\boldsymbol{\epsilon}}(t_n)$.
 338 In (44), values for \mathbf{S}_{τ_s} and $\tilde{\mathbf{S}}^v$ are taken for half the time increment, e.g. $\mathbf{S}_{\tau_s}|_{1/2} =$
 339 $(\mathbf{S}_{\tau_s}(t_n) + \mathbf{S}_{\tau_s}(t_{n+1}))/2$. The evolution laws for $\boldsymbol{\xi}$ and $\boldsymbol{\beta}_{\tau_s}$ are the same as in section
 340 3, see eq.(16). Similarly, the macroscopic thermoelastic strain given in equation (19) is
 341 computed using

$$342 \quad \Delta \tilde{\boldsymbol{\epsilon}}_0 = \left\langle {}^T \mathbf{B}_r^e : \Delta \boldsymbol{\epsilon}_{0r} - \sum_s {}^T \mathbf{B}_{r\tau_s} : \Delta \boldsymbol{\eta}_{r\tau_s} \right\rangle \quad (45)$$

343 and the phase average stress

$$\begin{aligned} 344 \quad \Delta \langle \boldsymbol{\sigma} \rangle_r &= \mathbf{B}_r^e : \Delta \bar{\boldsymbol{\sigma}} - \sum_s \mathbf{B}_{r\tau_s} |_{1/2} : \Delta \boldsymbol{\beta}_{\tau_s} + \mathbf{D}_r^e : (\Delta \tilde{\boldsymbol{\epsilon}}_0 - \Delta \boldsymbol{\epsilon}_{0r}) - \\ 345 \quad &\sum_s \mathbf{D}_{r\tau_s} |_{1/2} : (\Delta \boldsymbol{\theta}_{\tau_s} - \Delta \boldsymbol{\eta}_{r\tau_s}) \end{aligned} \quad (46)$$

344 where the new macroscopic internal variable $\boldsymbol{\theta}_{\tau_s} = \boldsymbol{\lambda}_{r\tau_s} + \boldsymbol{\eta}_{r\tau_s}$ is introduced for numerical
 345 purpose (see Appendix B)

$$346 \quad \dot{\boldsymbol{\theta}}_{\tau_s}(t) + \frac{1}{\tau_s} \boldsymbol{\theta}_{\tau_s}(t) = \frac{1}{\tau_s} \tilde{\boldsymbol{\epsilon}}_0(t) , \quad \boldsymbol{\theta}_{\tau_s}(0) = \mathbf{0}. \quad (47)$$

347 Phase average strain increments can then be computed with (41). Note that if hardening
 348 is discarded ($c = d = e = H = 0$), behaviors given by (44) and (14) are strictly
 349 equivalent.

350 When used with the original integral approach, the standard collocation method
 351 applied to polycrystals with local behavior (35-40) requires calculation of coefficients

352 \mathbf{S}_{τ_s} at each time step. This is also the case for the proposed incremental approach.
 353 However, unlike the present formulation, the integral approach requires keeping record
 354 of the whole history of $\tilde{\mathbf{S}}$ and \mathbf{B}_r from the very first loading stage for the evaluation of
 355 integrals (9), which is cumbersome especially when dealing with polycrystals with a large
 356 number of mechanical phases and loading steps. With the proposed approach (denoted
 357 Incremental Collocation Method, ICM), the numerical resolution is incremental. A step-
 358 by-step procedure can be applied, in which the aim of internal variables is to summarize
 359 the effects of the whole stress and strain history. This allows studying the polycrystal
 360 response for any complex loading with much more ease and flexibility. The algorithm
 361 for numerical implementation of the ICM is detailed in Appendix B.

362 4.3. Application

363 To show the potentiality of the proposed ICM, the microstructure introduced in section
 364 3.4 is investigated for deformation under the complex loading (34). Results are compared
 365 with reference solutions generated by the full-field FFT method, as in section 3. The
 366 local behavior (35-40) has been implemented with coefficients indicated in Table 1 and
 367 $\dot{\gamma}_0 = 1\text{s}^{-1}$, $m = 1$, and $H^{(k,l)} = 2 \forall k, l$. Figure 4 shows the effective stress response
 368 for two cases: (i) when both isotropic and kinematic are considered (with parameters
 369 $c = 5\text{MPa}$, $d = 10$, $e = 0$), and (ii) with isotropic hardening only ($c = d = e = 0$).
 370 It can be seen that, for both cases, the ICM matches well FFT solutions at the very
 371 first loading stage, but then the effective behavior becomes softer than the FFT one,
 372 the largest stress discrepancy $\bar{\sigma}_{13}^{\text{FFT}} - \bar{\sigma}_{13}^{\text{INC}}$ being observed close to the stress peak
 373 $t \approx 1\text{s}$. At larger time after several loading cycles, the discrepancy decreases until both
 374 responses coincide again.

375 It is recalled that the step-by-step numerical resolution of the ICM provides the
 376 same results as the internal variable approach of section 3 when hardening is discarded.
 377 Therefore, observed discrepancies are associated with the treatment of hardening. This
 378 is now illustrated with the case for which only isotropic hardening has been considered.
 379 Here, the main difference with results presented in section 3 is that $\tau_0^{(k)}$ is evolving. As
 380 discussed above, $\dot{\gamma}^{(k)}(\mathbf{x})$ had to be replaced by $\langle \dot{\gamma}^{(k)} \rangle_r$ in the hardening law for the ICM
 381 to be solved with standard mean-field homogenization techniques. Hence, instead of
 382 correctly predicting intraphase fluctuations for $\tau_0^{(k)}$ as with the FFT approach, the ICM
 383 requires phase uniform values. Consequences of this limitation have been investigated
 384 in [33] for viscoplastic polycrystals. Here, the ICM underestimates the average value of
 385 $\langle \tau_0^{(k)} \rangle_r$ compared to FFT reference results. At the same time, the overall behavior for
 386 the ICM is softer than for FFT predictions; this can originate from lower $\langle \tau_0^{(k)} \rangle_r$ but
 387 also from the intraphase heterogeneity of $\tau_0^{(k)}$, not predicted by ICM. Figure 5a shows
 388 an example of result for slip system $k = 1$ of phase $r = 1$ (similar trend is observed
 389 for other slips systems). Interestingly, the stress discrepancy $\bar{\sigma}_{13}^{\text{FFT}} - \bar{\sigma}_{13}^{\text{INC}}$ is found to
 390 be correlated with the standard deviation $\sqrt{\langle \tau_0^{(k)} \tau_0^{(k)} \rangle - \langle \tau_0^{(k)} \rangle^2}$ (computed with

Table 1. Parameters of the constitutive relation.

Slip system k	μ_e [MPa]	$\tau_0(t=0)$ [MPa]	τ_{sta} [MPa]
1	1	2	4
2	100	20	30

391 FFT) of $\tau_0^{(k)}$. As shown in figure 5b, the highest stress discrepancy at stress peak
 392 coincides with the largest standard deviation. Then, as the number of loading cycles
 393 increases, $\langle \tau_0^{(k)} \rangle_r$ becomes closer to the stationary value and at the same time $\tau_0^{(k)}$
 394 becomes more uniform within phases. At large time, ICM and FFT predictions coincide
 395 again.

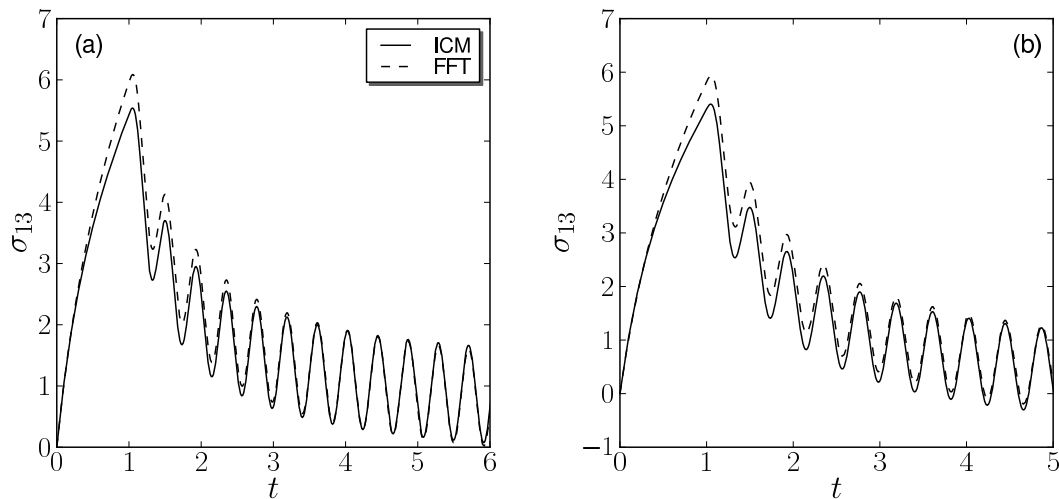


Figure 4. Viscoelastic homogenization with (a) both isotropic and kinematic hardening and (b) isotropic hardening only. Comparisons between incremental collocation and FFT methods for the macroscopic stress response $\bar{\sigma}_{13}$.

396 5. Concluding remarks

397 In the present article, the equivalence between the collocation method used to inverse
 398 Laplace-Carson transforms and an internal variables formulation has been developed
 399 for the case of linear thermo-viscoelastic polycrystalline materials exhibiting general
 400 anisotropic properties for local and macroscopic behaviors. The method has been
 401 applied to 2-D polycrystals with 2 slip systems per phase, deformed under antiplane
 402 shear, for macroscopic loading including stress discontinuities and for complex strain
 403 loading including a cyclic stage. It has been shown that the internal variable method
 404 yields accurate results that perfectly match the standard collocation method. Excellent
 405 agreement has also been obtained with references solutions provided by the full-field FFT
 406 numerical scheme. The formulation has been extended to the case of time- and strain-

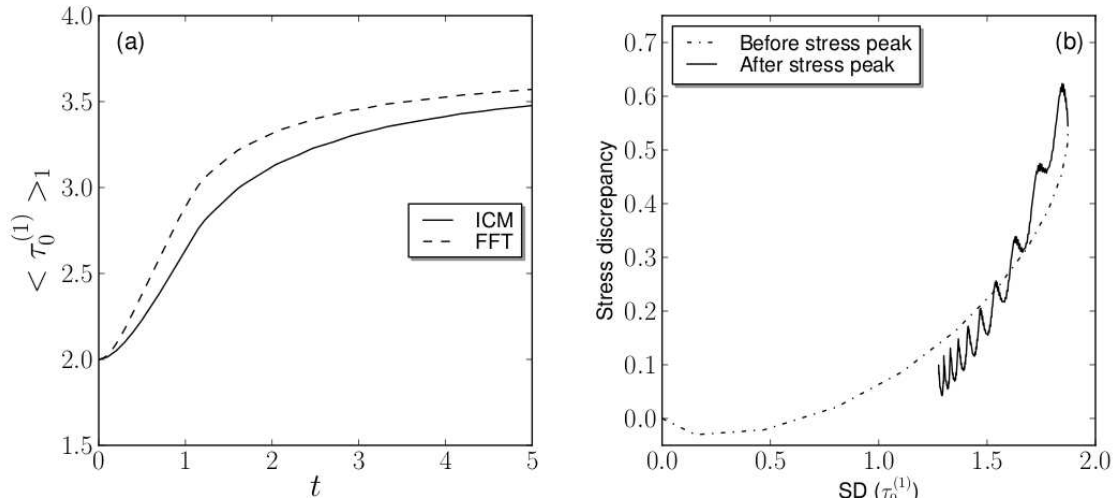


Figure 5. Viscoelastic homogenization with isotropic hardening predicted by the incremental collocation and FFT methods. (a) Evolution of $\langle \tau_0^{(1)} \rangle_1$. (b) Difference between the overall stresses $\bar{\sigma}_{13}$ obtained with FFT and ICM as a function of the standard deviation of $\tau_0^{(1)}$.

407 dependent constitutive viscous properties. In that case, an incremental collocation
 408 method is proposed. It can be efficiently solved numerically using a step-by-step
 409 procedure, and a general algorithm has been proposed. The capability of the method has
 410 been illustrated on a 2-D polycrystal, but it is worth noting that solving similar problems
 411 with 3-D polycrystals exhibiting few thousand phases requires only a few minutes on a
 412 standard laptop. The new method is therefore especially efficient for solving complex
 413 loading paths. Moreover, the introduction of isotropic and kinematic hardening at the
 414 slip system level has been considered. Some discrepancies with reference FFT results
 415 have been observed. They are likely due to the approximation made in considering phase
 416 uniform hardening variables within mean-field homogenization. Finally, it is pointed
 417 out that the obtained ICM offers a simple framework to address the case of nonlinear
 418 behaviors, e.g. using a linearization procedure similar as the one proposed by [21].

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 422 Cadarache, France) for stimulating discussions on the subject.

423 Appendix A. Relaxation function for an anisotropic Maxwell behavior

424 For general anisotropy, tensors \mathbf{C} and \mathbf{S} verify

$$425 \quad \mathbf{C} \star \mathbf{S} = \mathbf{I}, \quad \mathbf{C}^* : \mathbf{S}^* = \mathbf{I}. \quad (\text{A.1})$$

426 For a Maxwell behaviour, the creep function is $\mathbf{S}(t) = \mathbf{S}^e + \mathbf{S}^v t$ and the LC transform
427 of the relaxation function thus reads

$$428 \quad \mathbf{C}^*(p) = \left(\mathbf{S}^e + \frac{1}{p} \mathbf{S}^v \right)^{-1}. \quad (\text{A.2})$$

429 For general anisotropy, an analytic expression for the relaxation function $\mathbf{C}(t)$, given
430 by the inverse transform of \mathbf{C}^* , cannot be obtained. However, a closed-form expression
431 can be found for particular symmetry classes by using the spectral decomposition of the
432 fourth-order symmetric tensors [34]. For an isotropic behaviour, local properties read

$$433 \quad \mathbf{S}^e = \frac{1}{3k^e} \mathbf{J} + \frac{1}{2\mu^e} \mathbf{K}, \quad \mathbf{S}^v = \frac{1}{3k^v} \mathbf{J} + \frac{1}{2\mu^v} \mathbf{K} \quad (\text{A.3})$$

434 and thus

$$435 \quad \mathbf{C}^*(p) = 3k^e \left(\frac{\tau_k p}{1 + \tau_k p} \right) \mathbf{J} + 2\mu^e \left(\frac{\tau_\mu p}{1 + \tau_\mu p} \right) \mathbf{K} \quad (\text{A.4})$$

436 with $\tau_k = k^v/k^e$ and $\tau_\mu = \mu^v/\mu^e$ two characteristic relaxation times. The corresponding
437 relaxation function is given by

$$438 \quad \mathbf{C}(t) = 3k^e \exp(-t/\tau_k) \mathbf{J} + 2\mu^e \exp(-t/\tau_\mu) \mathbf{K}. \quad (\text{A.5})$$

439 For cubic symmetry, the local properties read

$$440 \quad \mathbf{S}^e = \frac{1}{3k^e} \mathbf{J} + \frac{1}{2\mu_a^e} \mathbf{K}_a + \frac{1}{2\mu_b^e} \mathbf{K}_b, \quad \mathbf{S}^v = \frac{1}{3k^v} \mathbf{J} + \frac{1}{2\mu_a^v} \mathbf{K}_a + \frac{1}{2\mu_b^v} \mathbf{K}_b \quad (\text{A.6})$$

441 and thus

$$442 \quad \mathbf{C}^*(p) = 3k^e \left(\frac{\tau_k p}{1 + \tau_k p} \right) \mathbf{J} + 2\mu_a^e \left(\frac{\tau_{\mu_a} p}{1 + \tau_{\mu_a} p} \right) \mathbf{K}_a + 2\mu_b^e \left(\frac{\tau_{\mu_b} p}{1 + \tau_{\mu_b} p} \right) \mathbf{K}_b \quad (\text{A.7})$$

443 with $\tau_k = k^v/k^e$, $\tau_{\mu_a} = \mu_a^v/\mu_a^e$ and $\tau_{\mu_b} = \mu_b^v/\mu_b^e$ three characteristic relaxation times.
444 The corresponding relaxation function thus reads

$$445 \quad \mathbf{C}(t) = 3k^e \exp(-t/\tau_k) \mathbf{J} + 2\mu_a^e \exp(-t/\tau_{\mu_a}) \mathbf{K}_a + 2\mu_b^e \exp(-t/\tau_{\mu_b}) \mathbf{K}_b. \quad (\text{A.8})$$

446 Similar expressions can be obtained for other symmetry classes.

447 **Appendix B. Numerical resolution of the incremental collocation method**

448 We provide here the algorithm for the step-by-step resolution of the ICM described in
449 section 4. The case of loadings with prescribed $\bar{\boldsymbol{\sigma}}$ is presented first. Assuming that
450 the homogenization problem has been solved for times $0 \leq t \leq t_n$, we seek to find
451 the mechanical response at time t_{n+1} associated to stress and time increments $\Delta \bar{\boldsymbol{\sigma}}$ and
452 Δt . The algorithm consists essentially of 3 loops, besides the time loop: the outer loop
453 (index i) for solving $\tilde{\boldsymbol{\varepsilon}}_0$ and \mathbf{S}^v , the inner loop (index j) for $\Delta \boldsymbol{\sigma}_r$, and a loop for the
454 symbolic homogenization problem.

455 (1) Computation of $\Delta \boldsymbol{\beta}_{\tau_s}$ and $\Delta \boldsymbol{\xi}$ following (16)

456 (2) Initializations: $(\mathbf{S}^v)_{t_{n+1}}^{i=0} = (\mathbf{S}^v)_{t_n}$; $(\mathbf{S}_{\tau_s})_{t_{n+1}}^{i=0} = (\mathbf{S}_{\tau_s})_{t_n}$; $(\tilde{\mathbf{S}}^v)_{t_{n+1}}^{i=0} = (\tilde{\mathbf{S}}^v)_{t_n}$; $(\mathbf{B}_{r_{\tau_s}})_{t_{n+1}}^{i=0} =$
457 $(\mathbf{B}_{r_{\tau_s}})_{t_n}$; $(\mathbf{D}_{r_{\tau_s}})_{t_{n+1}}^{i=0} = (\mathbf{D}_{r_{\tau_s}})_{t_n}$

- 458 (3) Computation of $\Delta \langle \boldsymbol{\sigma} \rangle_r$:
- 459 (a) Initialization of $(\Delta \langle \boldsymbol{\sigma} \rangle_r)^{j=0}$
- 460 (b) Computation of $(\Delta X)^j$ and $(\Delta \tau_0)^j$ following (39-40)
- 461 (c) Computation of $(\Delta \boldsymbol{\varepsilon}_{0r})^j$ and $(\Delta \langle \boldsymbol{\varepsilon} \rangle_r)^j$ following (42-41)
- 462 (d) Computation of $(\Delta \boldsymbol{\eta}_{r\tau_s})^j$ following (20)
- 463 (e) Computation of $(\Delta \tilde{\boldsymbol{\varepsilon}}_0)^j$ following (45)
- 464 (f) Computation of $(\Delta \boldsymbol{\theta}_{\tau_s})^j$ following (47)
- 465 (g) Actualization of $(\Delta \langle \boldsymbol{\sigma} \rangle_r)^{j+1}$ following (46)
- 466 (h) Compute convergence error $\boldsymbol{\delta}_1 = |(\Delta \langle \boldsymbol{\sigma} \rangle_r)^{j+1} - (\Delta \langle \boldsymbol{\sigma} \rangle_r)^j|$
- 467 If $\boldsymbol{\delta}_1 < \text{threshold}$ then go to (4), else $j \leftarrow j + 1$ and return to (3.b)
- 468 (4) Actualization of $(\tilde{\boldsymbol{\varepsilon}}_0)_{t_{n+1}}^{i+1}$ and $(\mathbf{S}^v)_{t_{n+1}}^{i+1}$ following (42)
- 469 (5) Homogenization of the symbolic thermo-elastic problem $\Rightarrow (\mathbf{S}_{\tau_s})_{t_{n+1}}^{i+1}; (\tilde{\mathbf{S}}^v)_{t_{n+1}}^{i+1};$
- 470 $(\mathbf{B}_{r\tau_s})_{t_{n+1}}^{i+1}; (\mathbf{D}_{r\tau_s})_{t_{n+1}}^{i+1}$
- 471 (6) Compute convergence error $\boldsymbol{\delta}_2 = |(\mathbf{S}^v)_{t_{n+1}}^{i+1} - (\mathbf{S}^v)_{t_{n+1}}^i|$
- 472 If $\boldsymbol{\delta}_2 < \text{threshold}$ then go to (7), else $i \leftarrow i + 1$ and return to (3.b)
- 473 (7) Output macroscopic and local responses at time t_{n+1} , and go to (2) for the next
- 474 time step

475 In cases of loading with prescribed $\bar{\boldsymbol{\varepsilon}}$ (instead of $\bar{\boldsymbol{\sigma}}$ as above), the algorithm has to

476 be slightly changed since $\Delta \boldsymbol{\beta}_{\tau_s}$ and $\Delta \boldsymbol{\xi}$ cannot be calculated in advance.

- 477 (1) Initializations: $(\mathbf{S}^v)_{t_{n+1}}^{i=0} = (\mathbf{S}^v)_{t_n}; (\mathbf{S}_{\tau_s})_{t_{n+1}}^{i=0} = (\mathbf{S}_{\tau_s})_{t_n}; (\tilde{\mathbf{S}}^v)_{t_{n+1}}^{i=0} = (\tilde{\mathbf{S}}^v)_{t_n}; (\mathbf{B}_{r\tau_s})_{t_{n+1}}^{i=0} =$
- 478 $(\mathbf{B}_{r\tau_s})_{t_n}; (\mathbf{D}_{r\tau_s})_{t_{n+1}}^{i=0} = (\mathbf{D}_{r\tau_s})_{t_n}$
- 479 (2) Computation of $\Delta \boldsymbol{\beta}_{\tau_s}, \Delta \boldsymbol{\xi}$ and $\tilde{\boldsymbol{\varepsilon}}_0$
- 480 (a) Initialization : $(\Delta \boldsymbol{\beta}_{\tau_s})^j = (\Delta \boldsymbol{\beta}_{\tau_s})^0, (\Delta \boldsymbol{\xi})^j = (\Delta \boldsymbol{\xi})^0$ and $(\Delta \tilde{\boldsymbol{\varepsilon}}_0)^j = (\Delta \tilde{\boldsymbol{\varepsilon}}_0)^0$
- 481 (b) Computation of $(\Delta \bar{\boldsymbol{\sigma}})^j$ from (44)
- 482 (c) Computation of $(\Delta \boldsymbol{\beta}_{\tau_s})^{j+1}$ and $(\Delta \boldsymbol{\xi})^{j+1}$ following (16)
- 483 (d) Computation of $(\Delta \tilde{\boldsymbol{\varepsilon}}_0)^{j+1}$
- 484 1. Initialization of $(\Delta \langle \boldsymbol{\sigma} \rangle_r)^{k=0}$
- 485 2. Computation of $(\Delta \langle \boldsymbol{\sigma} \rangle_r)^{k+1}$ with steps (3.b) to (3.g) above
- 486 3. Compute convergence error $\boldsymbol{\delta}_1 = |(\Delta \langle \boldsymbol{\sigma} \rangle_r)^{k+1} - (\Delta \langle \boldsymbol{\sigma} \rangle_r)^k|$
- 487 If $\boldsymbol{\delta}_1 < \text{threshold}$ then $(\Delta \tilde{\boldsymbol{\varepsilon}}_0)^{j+1} = (\Delta \tilde{\boldsymbol{\varepsilon}}_0)^k$ and go to (2.e), else $k \leftarrow k + 1$
- 488 and return to (2.d.2)
- 489 (e) Compute convergence error $\boldsymbol{\delta}_2$ as the max of normalized value of
- 490 $|(\Delta \boldsymbol{\beta}_{\tau_s})^{j+1} - (\Delta \boldsymbol{\beta}_{\tau_s})^j|, |(\Delta \boldsymbol{\xi})^{j+1} - (\Delta \boldsymbol{\xi})^j|,$ and $|(\Delta \tilde{\boldsymbol{\varepsilon}}_0)^{j+1} - (\Delta \tilde{\boldsymbol{\varepsilon}}_0)^j|$
- 491 If $\boldsymbol{\delta}_2 < \text{threshold}$ then go to (3), else $j \leftarrow j + 1$ and return to (2.b)
- 492 (3) Reactualization of $(\mathbf{S}^{vsct})_{t_{n+1}}^{i+1}$ following (??)
- 493 (4) Homogenization of the symbolic thermo-elastic problem $\Rightarrow (\mathbf{S}_{\tau_s})_{t_{n+1}}^{i+1}; (\tilde{\mathbf{S}}^v)_{t_{n+1}}^{i+1};$
- 494 $(\mathbf{B}_{r\tau_s})_{t_{n+1}}^{i+1}; (\mathbf{D}_{r\tau_s})_{t_{n+1}}^{i+1}$
- 495 (5) Compute convergence error $\boldsymbol{\delta}_3 = |(\mathbf{S}^v)_{t_{n+1}}^{i+1} - (\mathbf{S}^v)_{t_{n+1}}^i|$
- 496 If $\boldsymbol{\delta}_3 < \text{threshold}$ then go to (6), else $i \leftarrow i + 1$ and return to (2)

- 497 (6) Output macroscopic and local responses at time t_{n+1} , and go to (2) for the next
498 time step

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