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Building of a reduced constitutive law for ceramic matrix composites

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Abstract

The aim of this paper is to set up a methodology in order to build a reduced constitutive law in case of a complex material behavior. The reduction is performed in a certain range of loading conditions in order to preserve the state potential describing the original complex model. Two main steps are used. The first one concerns the reduction of the kinematic of the internal variables from which associated thermodynamical forces are deduced. In order to define the internal variables, a simple thermodynamic potential form is chosen. The second concerns the building of the evolution laws linking the previous variables. The presented methodology has been applied to the mechanical modeling of SiC/SiC ceramic matrix composites.

Keywords: constitutive relation, Principal Component Analysis (PCA), reduced model, composite, anisotropic damage

1 INTRODUCTION

Some materials, like SiC / SiC ceramic matrix composites (SiC fibers in SiC matrix) exhibit very complex mechanical behaviors [Aubard et al., 1994]. For example, damage and inelasticity with closure effects when loading in compression, fatigue or damage anisotropy directed by the loading direction (i.e. not known a priori). Modeling such materials in a general manner leads to set up complex models [Ladevèze, 2002, Cluzel et al., 2009]. Such models can also be used for metals or concrete as in [Lemaitre and Desmorat, 2005]. However, using this kind of constitutive laws to simulate the mechanical behavior of a structure [Genet et al., 2011] can lead to very expensive computational costs even if the loading is locally simple. The aim of this paper is to set up a methodology in order to reduce such an existing law according to a certain range of loading conditions (monotonous, multi-axial proportional, constant temperature...). The reduced model will then be defined by a small set of internal variables and the associated evolution laws. Note that, the existence of a complex model prior to a simple one is due to the industrial context which is the following. The model has been first developed for military applications i.e. complex highly

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loaded structures. Now, applications are moving to civil applications [Bourgeon, 2010]. In order to improve the lifetime of the material, the civil loading range is only a subset of the military loading range (mainly lower stress levels). Therefore, in that last range of loadings, a more simple model is sufficient to describe the behavior of the material. A loading range is, in this paper, the set of all admissible loading conditions mainly defined by maximum stress levels and loading histories (uniaxial, multiaxial, proportional, monotonous, cyclic...). For example, while for a military application a stress up to 200 MPa can be considered, for civil applications only 100 MPa are considered.

Two main approaches can be applied for that purpose. The first one consists in directly modeling the mechanical behavior from a reduced set of experimental data. Some information are then lost. The second consists in building the response surface linking directly the stress field to the strain field. This approach does not rely on the physics of the material and may be unable to describe unloading/loading cycles. In the approach proposed in the present paper, different laws can be deduced from a physical model depending on the chosen subset of loading conditions. Nevertheless, the objective is to get one reduced model for a set of applications and not to deal with different reduced models on different locations of the structure. The reduced model is compatible with the original one and the original model can still be used on some points of difficulty as the limits of the reduced model are known and can be evaluated. The simplified model can be used in standard finite element codes as a user material behavior. The reduced model concerns, in this paper, a constitutive law. This law must be in a form adapted to classical finite element codes and implementable in a material user subroutine. It is thus different from structural model reduction techniques like Proper Generalized Decomposition (a review on PGD can be found in [Chinesta et al., 2011]) or other Proper Orthogonal Decomposition (POD) techniques (a review can be found in [Ryckelynck et al., 2006]) like model hyper-reduction [Ryckelynck, 2009]. Indeed, the objective of these techniques is to compress information in order to speed up structural computations. The compressed information is generally the evolution of the displacement field. Thus, these strategies need to perform operations over the whole space and time domains.

The proposed approach relies on the classical modeling framework: the thermodynamics of irreversible processes with internal variables [Nguyen et al., 1983, Lemaitre, 1992]. The different steps are:

1. Choice of the state variables and of a potential (the interpretation of the variables is given by the potential form);
2. Computation of the associated thermodynamical forces by duality with state variables;
3. Computation of the state laws;
4. Definition of the evolution laws.

Considering the objective of simplifying an existing model, the value of the thermodynamical potential is known (or can be computed) for a certain load history. This paper will then focus on defining new state variables (and deduce their associated forces) and the evolution laws. In order to illustrate the present strategy, this paper will focuss on an anisotropic modeling of ceramic matrix composites developed in [Ladevèze, 2002, Cluzel et al., 2009, Genet et al., 2011].

2 MODELING OF CERAMIC MATRIX COMPOSITES MECHANICAL BEHAVIOR

Ceramic matrix composites present a non-linear mechanical behavior up to rupture although both constituents (fibre and matrix) are brittle. This is due to the presence of an interface between the fibers and the matrix, usually pyrocarbon (PyC) that deflects the cracks along the fibre. Various degradation mechanisms are evidenced until failure through a scenario as summarize in [Lamon, 2001]: (i) initiation of cracks at macropores, (ii) inter-yarn transverse cracks, (iii) longitudinal transverse cracks. The cracks are deviated at the yarn/matrix interface (inter-yarn cracks) or at the fibre/matrix interface (intra-yarn cracks). Note that inter-yarn transverse cracks are mainly directed by the loading direction (a priori unknown) and that crack closure may have a significant effect and the mechanical behaviour. The cracks opening are a preferential path for the oxygen diffusion that reduces the strength of the SiC fibers.

The mechanical model takes into account the crack networks and the associated fiber-matrix debonding through damage and inelastic strains. The inelastic part being relatively classical, it is not presented here nor treated in the model reduction for the sake of simplicity. The damage part is based on anisotropic and unilateral damage theory, a powerful damage approach introduced in [Ladevèze, 1983, Ladevèze, 2002] and previously applied to SiC/SiC [Aubard et al., 1998, Gasser et al., 1996] composites and to concrete [Desmorat et al., 2007]. The first version of the theory used second-order tensors to represent mechanical damage [Ladevèze, 1983]. It was superseded by a second version which uses fourth-order tensors [Ladevèze, 2002]. The same choice was also made by [Lesne and Saanouni, 1993, Voyiadjis and Kattan, 1993]. The unilateral character of damage (which, under compression loading, is passive) is taken into account without resorting to a discontinuous state law. This property is also present, in a different form, in [Pensée et al., 2002, Chaboche and Maire, 2002, Marcin et al., 2010]. Finally, the approach has the particularity of treating each damage mechanism (inter-yarn cracking, intra-yarn longitudinal cracking and intra-yarn transversal cracking) separately. The main constitutive equations, as implemented in the finite element industrial code Abaqus/Standard, will now be reviewed.

The potential of elastic energy density is expressed in terms of the stress tensor $\boldsymbol{\sigma}$ and divided into three parts: (i) a first part which is active only in traction and which takes into account the damage state, (ii) a second part which is active only in compression and which is independent of the damage state and (iii) a third part which is always active and also involves some damage. Thus, this potential can be expressed as:

$$e_d = \frac{1}{2}Tr[\mathbb{C}\boldsymbol{\sigma}^+\boldsymbol{\sigma}^+] + \frac{1}{2}Tr[\mathbb{C}_0\boldsymbol{\sigma}^-\boldsymbol{\sigma}^-] + \frac{1}{2}Tr[\mathbb{Z}\boldsymbol{\sigma}\boldsymbol{\sigma}] \quad (1)$$

where \mathbb{C}_0 , \mathbb{C} and \mathbb{Z} are three fourth-order tensors representing respectively the initial compliance, the damaged compliance and a compliance operator associated with shear damage. In addition, a special decomposition of the stress tensor into a positive part and a negative part is used in order to ensure the continuity of the state law [Ladevèze, 2002]:

$$\begin{cases} \boldsymbol{\sigma}^+ = \mathbb{C}^{-1/2} : \langle \mathbb{C}^{1/2} : \boldsymbol{\sigma} \rangle_+ \\ \boldsymbol{\sigma}^- = \mathbb{C}_0^{-1/2} : \langle \mathbb{C}_0^{1/2} : \boldsymbol{\sigma} \rangle_- \end{cases} \quad (2)$$

where $\langle \rangle_{+/-}$ denotes the classical positive and negative parts of the quantities being considered.

It is important to remember that both the positive part and the negative part must be taken in that special sense (and not in the classical sense) in order to avoid a discontinuous state law.

Thus, the state law becomes:

$$\boldsymbol{\epsilon}^e = \frac{\partial e_d}{\partial \boldsymbol{\sigma}} = \mathbb{C}\boldsymbol{\sigma}^+ + \mathbb{C}_0\boldsymbol{\sigma}^- + \mathbb{Z}\boldsymbol{\sigma} \quad (3)$$

where $\boldsymbol{\epsilon}^e$ is the elastic strain tensor.

The energy release rates associated with the variations of internal variables \mathbb{C} and \mathbb{Z} , *i.e.* the thermodynamical forces, are:

$$\begin{cases} \mathbb{Y} = \frac{\partial e_d}{\partial \mathbb{C}} = \frac{1}{2}\boldsymbol{\sigma}^+ \otimes \boldsymbol{\sigma}^+ \\ \mathbb{Y}' = \frac{\partial e_d}{\partial \mathbb{Z}} = \frac{1}{2}\boldsymbol{\sigma} \otimes \boldsymbol{\sigma} \end{cases} \quad (4)$$

Finally, an additional thermodynamic force, which is required to drive shear damage correctly, is defined as:

$$\begin{aligned} \mathbb{Y}'' &= \frac{1}{2} (\mathbf{i}_{\pi/2}\boldsymbol{\sigma}^+)_{\text{sym}} \otimes (\mathbf{i}_{\pi/2}\boldsymbol{\sigma}^+)_{\text{sym}} \\ \text{with } \mathbf{i}_{\pi/2} &= \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \end{aligned} \quad (5)$$

Each degradation mechanism is associated with a damage evolution law which affects part or all of tensors \mathbb{C} and \mathbb{Z} :

$$\begin{cases} \dot{\mathbb{C}} = \dot{\mathbb{C}}_m + \dot{\mathbb{C}}_{f_1} + \dot{\mathbb{C}}_{f_2} \\ \dot{\mathbb{Z}} = \dot{\mathbb{Z}}_m + \dot{\mathbb{Z}}_{f_1} + \dot{\mathbb{Z}}_{f_2} \end{cases} \quad (6)$$

where $\dot{\mathbb{C}}_m$ and $\dot{\mathbb{Z}}_m$ represent inter-yarn matrix cracking, $\dot{\mathbb{C}}_{f_1}$ and $\dot{\mathbb{Z}}_{f_1}$ represent intra-yarn matrix cracking of the longitudinal tows, and $\dot{\mathbb{C}}_{f_2}$ and $\dot{\mathbb{Z}}_{f_2}$ represent intra-yarn matrix cracking of the transverse tows.

For instance, regarding inter-yarn matrix cracking, we consider the following effective thermodynamic force and its maximum over time:

$$\begin{cases} z_m = \left(a \text{Tr} [\widehat{\mathbb{Y}}]^{n+1} + (1-a) \text{Tr} [\widehat{\mathbb{Y}}^{n+1}] \right)^{1/n+1} \\ \bar{z}_m(t) = \sup_{\tau \leq t} z_m(\tau) \end{cases} \quad (7)$$

and the definition of the evolution law becomes:

$$\begin{cases} \dot{\mathbb{C}}_m = \dot{\alpha}_m \frac{a \left(\text{Tr} [\widehat{\mathbb{Y}}] \right)^n \mathbb{I} + (1-a) \widehat{\mathbb{Y}}^n}{\bar{z}_m^n} \\ \dot{\mathbb{Z}}_m = \dot{\alpha}_m \frac{b \widehat{\mathbb{Y}}''}{\bar{z}_m^n} \end{cases} \quad (8)$$

where $\dot{\alpha}_m$ is a function of \bar{z}_m which needs to be calibrated experimentally, and a , b , n are parameters of the model defining damage anisotropy (usually chosen as $a = 0.1$, $b = 2$ and $n = 2$).

The other damage evolution laws have similar expressions [Ladevèze, 2002]. The formulation for the transversal tow is similar [Letombe, 2005, Baranger et al., 2007]. Once again, for the sake of simplicity, the modeling of inelastic strains is not presented here. This is due to the friction between the fibers and the matrix when debonding occurs at fiber/matrix interphases. The associated models are up to now rather simple and do not need model reduction.

3 REDUCTION OF THE DAMAGE KINEMATICS: PRINCIPAL COMPONENT ANALYSIS (PCA)

Principal Component Analysis (PCA) is a very classical tool to analyse or compress statistical data. It is also well known as Proper Orthogonal Decomposition, Karhunen Loeve expansion, or Singular Value Decomposition in different scientific fields. It allows to find the best decomposition basis to represent a field for a given set of representative realizations of this field.

The potential reads:

$$e_d(\boldsymbol{\sigma}, \mathbb{C}, \mathbb{Z}) = \frac{1}{2} (Tr[\mathbb{C}\boldsymbol{\sigma}^+\boldsymbol{\sigma}^+] + Tr[\mathbb{C}_0\boldsymbol{\sigma}^-\boldsymbol{\sigma}^-] + Tr[\mathbb{Z}\boldsymbol{\sigma}\boldsymbol{\sigma}]) \quad (9)$$

The objective is to approximate this potential in the form of:

$$\tilde{e}_d(\boldsymbol{\sigma}, d_i) = \frac{1}{2} Tr\left[\left(\mathbb{C}_0 + \sum_i d_i \mathbb{C}_i\right) \boldsymbol{\sigma}\boldsymbol{\sigma}\right] \quad (10)$$

where $(d_i)_i$ is the new, reduced, set of damage variables. This potential still uses $\boldsymbol{\sigma}$ as state variable and is quite simple. In this approach, the form of the chosen potential is crucial because :

- it defines the meaning of the internal variables;
- it must be adapted to the complexity of the constitutive law to describe. If not adapted, the resulting reduced law may be inaccurate.

Note that, due to the simple form of the approximate potential, continuous damage evolution laws are sufficient to get continuous stress/strain relations.

Thus the principal component analysis will try to determine the best damage kinematic \mathbb{C}_i (these modes form an orthogonal basis) in a certain range of loadings, minimizing the error:

$$e^2 = \sum_{loads} Tr[\mathbb{C}_{err}\mathbb{C}_{err}] \quad (11)$$

This considers the sum of the errors on the load range accounted for the reduced model evaluation. The sum is therefore performed for all time steps for the different considered loading paths i.e. for each considered state of loading.

$$\mathbb{C}_{err} = (\mathbb{C}_0 + d_i \mathbb{C}_i) - \frac{\partial^2 e_d}{\partial \boldsymbol{\sigma}^2} \Big|_{damage} \quad (12)$$

This error compares the approximation of the compliance $\mathbb{C}_0 + d_i \mathbb{C}_i$ and the compliance of the original model. The term $\frac{\partial^2 e_d}{\partial \boldsymbol{\sigma}^2} \Big|_{damage}$ is the secant compliance compliance also noted $\frac{\partial \boldsymbol{\varepsilon}^e}{\partial \boldsymbol{\sigma}}$. Its computation is detailed in appendix A. It can be performed numerically or analytically.

The principal component analysis is performed on $\frac{\partial \boldsymbol{\varepsilon}^e}{\partial \boldsymbol{\sigma}} - \mathbb{C}_0$ that is some kind of damage compliance. The minimization classically reads (complements can be found in appendix B):

$$\min_{span(\mathbb{C}_i)} e^2 = \min_{span(\mathbb{C}_i)} \left(\sum_{loads} Tr[\mathbb{C}_{err}\mathbb{C}_{err}] \right) \quad (13)$$

$$= \min_{span(\mathbb{C}_i)} \left(- \sum_{loads} \sum_i d_i d_i \right) \quad (14)$$

$$= \max_{span(\mathbb{C}_i)} \left(\sum_{loads} \sum_i d_i d_i \right) \quad (15)$$

$$= \max_{span(\mathbb{C}_i)} \left(\sum_i \sum_{loads} \left(Tr \left[\left(\frac{\partial \epsilon^e}{\partial \sigma} - \mathbb{C}_0 \right) \mathbb{C}_i \right]^2 \right) \right) \quad (16)$$

$$= \max_{span(\mathbb{C}_i)} \sum_i \frac{Tr[\mathbb{C}_i (\sum_{loads} (\frac{\partial \epsilon^e}{\partial \sigma} - \mathbb{C}_0) \otimes (\frac{\partial \epsilon^e}{\partial \sigma} - \mathbb{C}_0)) \mathbb{C}_i]}{Tr[\mathbb{C}_i \mathbb{C}_i]} \quad (17)$$

The error is minimal for \mathbb{C}_i maximizing the Rayleigh quotient:

$$R(\mathbb{U}) = \frac{Tr[\mathbb{U} (\sum_{loads} (\frac{\partial \epsilon^e}{\partial \sigma} - \mathbb{C}_0) \otimes (\frac{\partial \epsilon^e}{\partial \sigma} - \mathbb{C}_0)) \mathbb{U}]}{Tr[\mathbb{U}\mathbb{U}]} \quad (18)$$

The set $(\mathbb{C}_i)_i$ is then obtained by solving the associated eigen-value problem. \mathbb{C}_i having the major and minor symmetries, this problem can be solved using matrix libraries and two successive Voigt notations. $(\mathbb{C}_i)_i$ are the eigenvectors and $(\alpha_i)_i$ the associated eigenvalues. This methodology as been applied to loading paths presented figure 1.

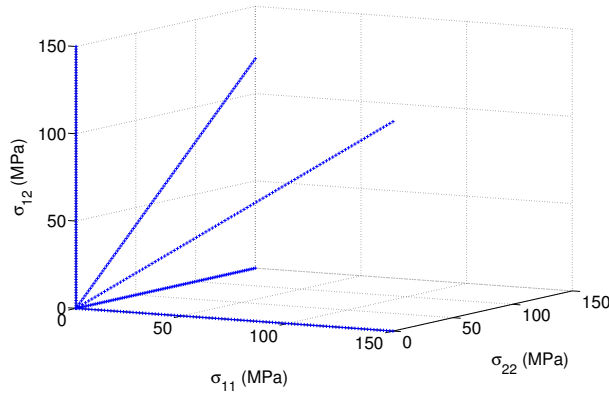


Figure 1: Loading paths for the reduced model construction

Six modes can be computed (in the Voigt notation), the percentage explained for each mode is presented in table 1. The chosen Voigt notation is the same for stress and strain $(\sigma_{11}, \sigma_{22}, \sqrt{2}\sigma_{12})$. The percentage explained of the mode i is given by: $\frac{\alpha_j}{\sum_j \alpha_j}$.

In table 2 are presented the modes of the PCA. The first one corresponds to the description of the shear while the second and third correspond to the description of the on-axis tractions.

Mode	1	2	3	4	5	6
% explained	94.7041	2.6930	2.3848	0.1991	0.0187	0.0002

Table 1: Percentage explained for each mode of the PCA.

\hat{C}_{11}	C_{1111}	0.1191	-0.6987	0.5923	-0.3674	0.1090	-0.0014
\hat{C}_{22}	C_{2222}	0.1191	0.6987	0.5923	-0.3674	-0.1090	-0.0014
\hat{C}_{33}	C_{1212}	0.9776	-0.0000	-0.2093	-0.0204	0.0000	-0.0042
$\sqrt{2}\hat{C}_{12}$	$\sqrt{2}C_{1122}$	0.0161	-0.0000	0.0474	0.0777	0.0000	0.9957
$\sqrt{2}\hat{C}_{13}$	$2C_{1112}$	0.0883	0.1090	0.3552	0.6015	0.6987	-0.0653
$\sqrt{2}\hat{C}_{23}$	$2C_{2212}$	0.0883	-0.1090	0.3552	0.6015	-0.6987	-0.0653

Table 2: Modes of the PCA.

The relative error on the potential can be computed for a truncated expansion, it is presented in table 3. Based on this table, one or two modes should be sufficient. Nevertheless, as the evolution law will be also approximated, the error will be greater. In practice, only the two first modes are retained.

Truncation order	1	2	3	4	5	6
% Error (%)	10	4.5	1.8	0.32	6E-3	0

Table 3: Relative error on the potential.

4 BUILDING OF THE DAMAGE EVOLUTION LAWS

The thermodynamical force associated to the damage variable d_i is:

$$y_i = \frac{\partial \tilde{e}_d}{\partial d_i} = \frac{1}{2} Tr[\mathbb{C}_i \boldsymbol{\sigma} \boldsymbol{\sigma}] \quad (19)$$

Thus, introducing the thermodynamical forces associated to \mathbb{C} and \mathbb{Z} (named \mathbb{Y} and \mathbb{Y}'), the computation of y_i is quite easy in Voigt notation.

$$y_i = Tr[\mathbb{C}_i \mathbb{Y}] \quad (20)$$

On figures 2 and 3 are presented the evolutions of the damage variables d_1 and d_2 versus the associated thermodynamical forces y_1 and y_2 for the considered range of loading. On that basis, approximated evolution laws have been identified and plotted on the same figures. Another way, more accurate but less efficient regarding the computational cost, is to build a response surface for each damage variable.

The evolutions laws are:

$$d_1 = \begin{cases} b_1 y_{eq}^2 & \text{if } y_{eq} < R \\ b_1 R^2 + b_2 (y_{eq} - R)^2 & \text{else} \end{cases} \quad (21)$$

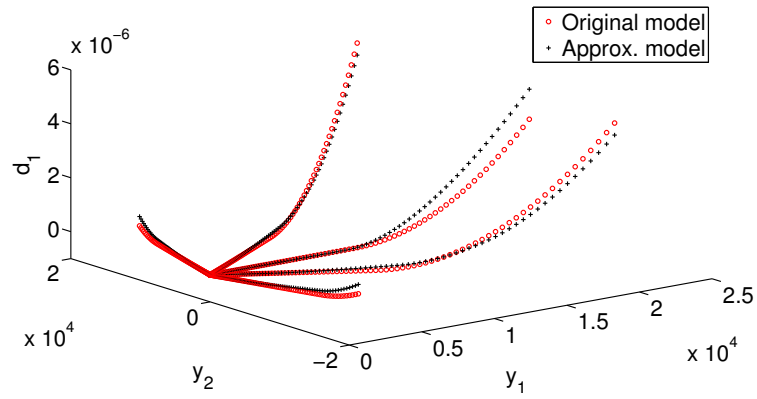


Figure 2: Evolution law for d_1

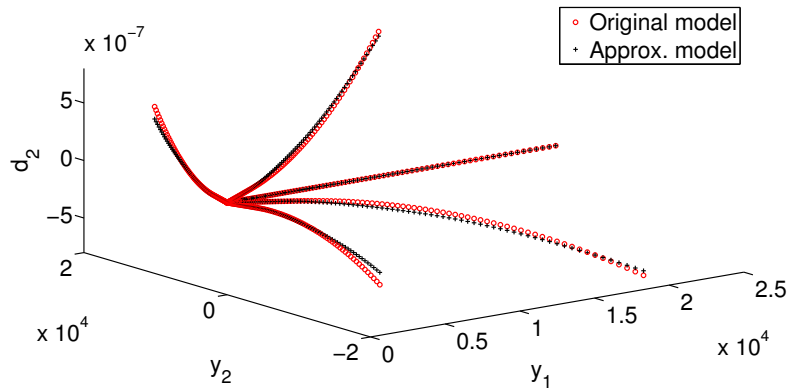


Figure 3: Evolution law for d_2

with the equivalent force:

$$y_{eq} = \sqrt{\left(\frac{y_1}{a_1}\right)^2 + \left(\frac{y_2}{a_2}\right)^2} \quad (22)$$

and:

$$d_2 = \begin{cases} a(y_2 - c)^2 & \text{if } y_2 > c \\ -a(y_2 + c)^2 & \text{if } y_2 < -c; \end{cases} \quad (23)$$

Note that if the kinematic of the model is not rich enough then the evolution laws may become quite complicated.

With the proposed evolution laws, the maximum relative error on the potential for the chosen range of loading is no more of 4.5% but reaches 20%. In fact, as it can be seen on figure 4, the error is of about 5% and greater for high shear loadings where the proposed evolution law of d_1 has the poorest approximation versus y_1 (20% error). On this figure, the different loading paths are presented sequentially (pure longitudinal loading from 0 to 100, pure transverse from 100 to 200, pure shear from 200 to 300, longitudinal and shear from 300 to 400, transverse and shear from 400 to 500). The abscissa is the time. This leads to a 12% relative error on the strain tensor components.

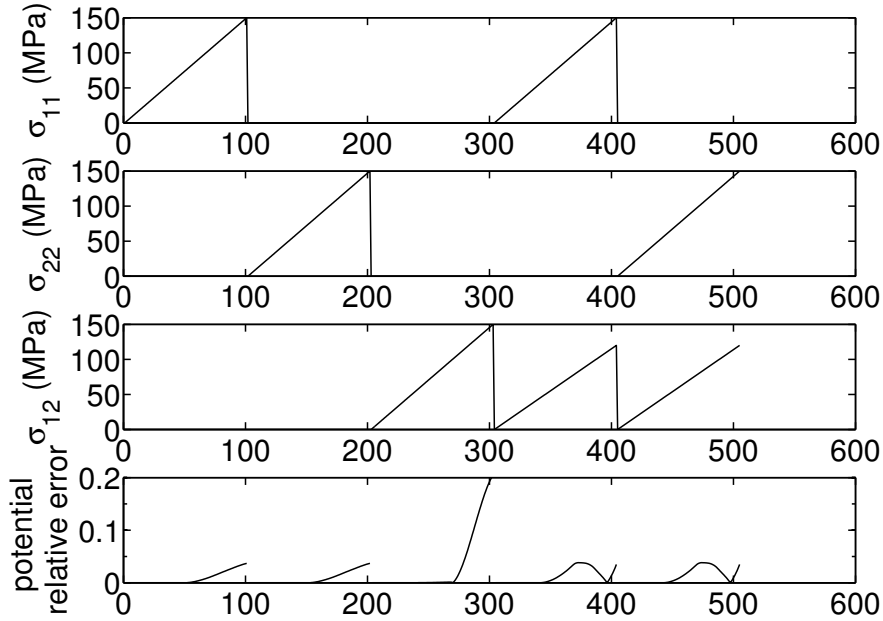


Figure 4: Localization of the relative error on the potential for the the studied loaded paths (presented sequentially)

The computational cost is greatly decreased using the reduced constitutive relation. For exam-

ple, for 505 runs covering the whole loading path set, the average cost ratio is:

$$\frac{cost_{original}}{cost_{reduced}} = 1500 \quad (24)$$

5 EVALUATION ON LARGER DIFFERENT LOADING PATHS

Figure 5 shows a wide range of loading paths examined to evaluate the capabilities of the model out of the construction range. Note that it is not the aim of such a construction.

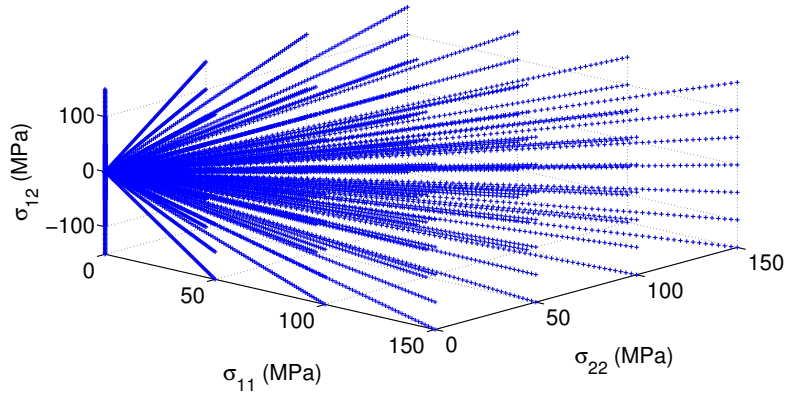


Figure 5: Extended loading paths

The previously computed damage modes are used for the projection of the damage variables and the definition of the thermodynamical forces. The figures 6 and 7 show the evolution of the damage variables, it can be seen that for some loadings, the form of the damage evolution laws are not accurate. This leads to incorrect values of the damage variables.

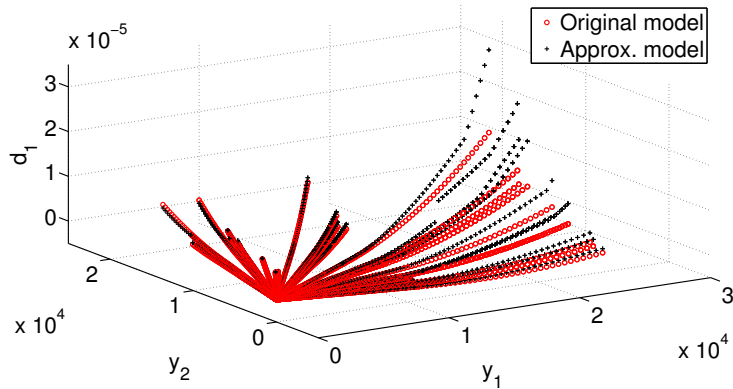


Figure 6: Evaluation of the evolution law for d_1

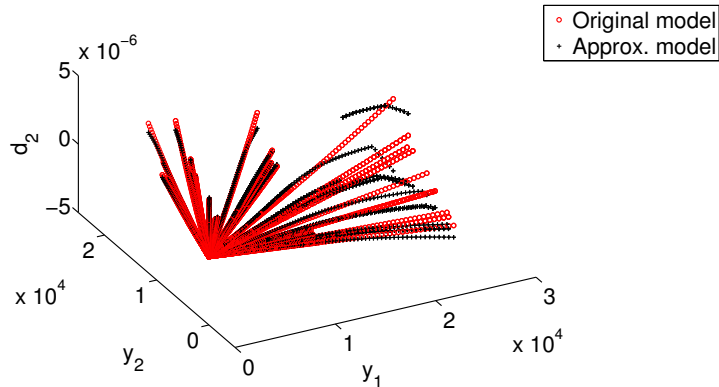


Figure 7: Evaluation of the evolution law for d_2

The maximum relative error on the potential is about 70% while the mean error is about 10%. On figure 8, the influence of the loading on the relative error on the potential is plotted. It can be seen that large errors are due to high shear loadings where the positive parts appearing in the original potential have an important role. On the strain components, the same relative error levels are observed.

Note that it is possible to include this large range of loadings at the beginning and to perform the complete analysis on that range. It leads to more complex evolution laws.

6 CONCLUSION AND OUTLOOKS

In this paper, a method enabling the reduction of a complex constitutive law is presented. It relies, first, on the proposition of an approximate potential form in order to introduce the reduced set of state variables. The second ingredient is the reduction of the state variables of the problem using a principal component analysis. From these newly defined damage variables, associated thermodynamical forces can easily be computed. The laws giving the evolution of the selected damage variables versus the associated thermodynamical forces are then classically identified but could also be modeled using a response surface. In the proposed range of loadings, the results are quite good and remain acceptable for a wider range of loading. The error between the original complex model and the approximation can be evaluated.

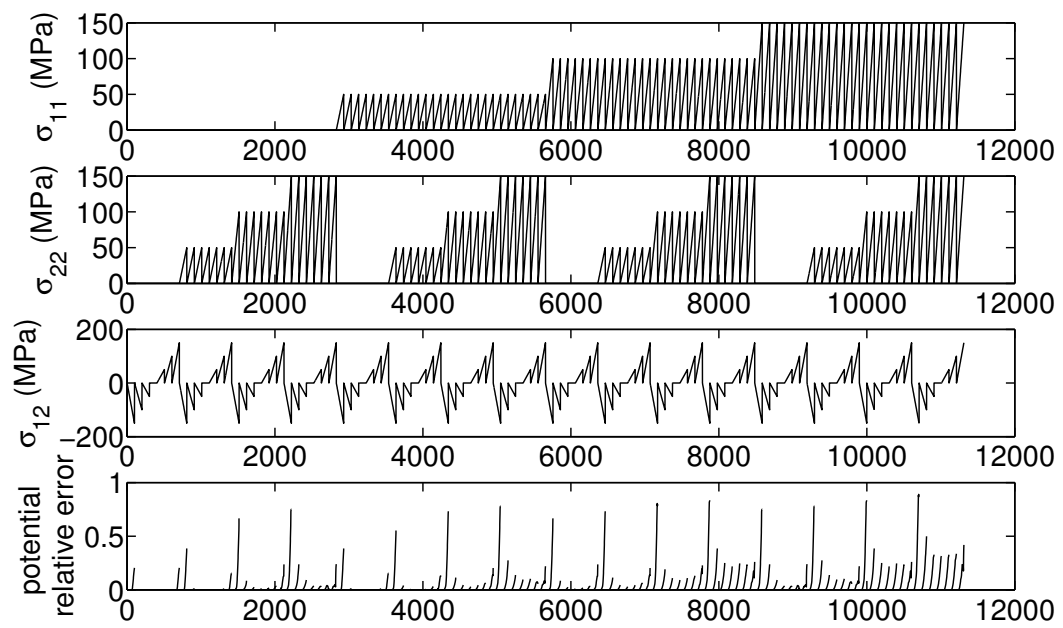


Figure 8: Localization of the relative error on the potential

A COMPUTATION OF $\frac{\partial \varepsilon^e}{\partial \sigma}$

The damage variables are assumed constant.

A.1 Definition of σ^+

σ^+ is defined using a generalized eigen-value problem.

\mathbb{H} definition An operator \mathbb{H} is introduced as the square root of \mathbb{C} .

$$\mathbb{C}\mathbf{A}_i = \lambda_i \mathbf{A}_i, \quad i \in [1, 3] \quad (25)$$

where \mathbf{A}_i is a symmetric second order tensor (because of the symmetries of \mathbb{C}). $(\mathbf{A}_i)_i$ are the Kelvin modes of \mathbb{C} .

$$Tr[\mathbf{A}_i \mathbf{A}_j] = \delta_{ij} \quad (26)$$

This lead to the decomposition of \mathbb{C} , starting from:

$$\mathbb{C}\mathbf{B} = \mathbb{C} \left(\sum_i \alpha_i \mathbf{A}_i \right) \quad (27)$$

with:

$$\alpha_i = Tr[\mathbf{A}_i \mathbf{B}]$$

Thus:

$$\mathbb{C}\mathbf{B} = \mathbb{C} \left(\sum_i \mathbf{A}_i Tr[\mathbf{A}_i \mathbf{B}] \right) \quad (28)$$

$$= \left(\sum_i \lambda_i \mathbf{A}_i Tr[\mathbf{A}_i \mathbf{B}] \right) \quad (29)$$

This is the Kelvin decomposition of \mathbb{C} .

\mathbb{H} is defined such as:

$$\mathbb{H}\mathbf{B} = \sum_i \lambda_i^{1/2} \mathbf{A}_i Tr[\mathbf{A}_i \mathbf{B}] \quad (30)$$

In Voigt notation:

$$\hat{H} = \sum_{i=1}^3 \lambda_i^{1/2} \hat{A}_i \hat{A}_i^T \quad (31)$$

So one have: $\hat{H}\hat{H} = \hat{C}$ and $\mathbb{H}\mathbb{H} = \mathbb{C}$.

Eigen-value problem and σ^+ Let introduce a spectral decomposition of σ using the following eigen-value problem:

$$\mathbb{H}\sigma T_i = \tilde{\lambda}_i T_i, \quad i \in [1, 2] \quad (32)$$

$\mathbb{H}\sigma$ is a symmetric second order tensor (due to the symmetries of \mathbb{H}). T_i is a vector.

$$\mathbb{H}\sigma = \sum_{i=1}^2 \tilde{\lambda}_i T_i T_i^T = \sum_i \tilde{\lambda}_i \sigma_i \quad (33)$$

where $\sigma_i = T_i T_i^T$, $i \in [1, 2]$.

Eigenvectors are orthogonal:

$$T_i^T T_j = \delta_{ij}$$

and

$$\sigma_i \sigma_j = T_i T_i^T T_j T_j^T = T_i T_j^T \delta_{ij}$$

thus $Tr[\sigma_i \sigma_j] = \delta_{ij}$, $(i, j) \in [1, 2]^2$.

The positive part is introduced as:

$$\langle \mathbb{H}\sigma \rangle_+ = \sum_i \lambda_i^+ T_i T_i^T = \sum_{i=1}^2 \lambda_i^+ \sigma_i \quad (34)$$

and

$$\sigma^+ = \mathbb{H}^{-1} \langle \mathbb{H}\sigma \rangle_+ \quad (35)$$

we have $\mathbb{H}^{-1} \mathbb{H} = \mathbb{I}_d$.

A.2 Variations calculus

variations of λ^+ We have

$$\lambda^+ = h(\lambda)\lambda \quad (36)$$

where h is the Heaviside function. Thus:

$$\delta(\lambda^+) = h(\lambda)\delta\lambda \quad (37)$$

variations of λ

$$\mathbb{H}\sigma T_i = \lambda_i T_i \quad (38)$$

Thus:

$$\mathbb{H}\delta\sigma T_i + \mathbb{H}\sigma\delta T_i = \delta\lambda_i T_i + \lambda_i \delta T_i \quad (39)$$

$$T_i^T \mathbb{H}\delta\sigma T_i + T_i^T \mathbb{H}\sigma\delta T_i = T_i^T \delta\lambda_i T_i + T_i^T \lambda_i \delta T_i \quad (40)$$

$$T_i^T \mathbb{H}\delta\sigma T_i = \delta\lambda_i \quad (41)$$

$$Tr[\sigma_i \mathbb{H}\delta\sigma] = \delta\lambda_i \quad (42)$$

from the orthogonality of the modes T_i , we also deduce the expression:

$$T_j^T \delta T_i = 0 \quad \forall i, j \quad (43)$$

A.3 Partial derivatives of the potential

Expression of the potential

$$Tr[\mathbf{C}\boldsymbol{\sigma}^+\boldsymbol{\sigma}^+] = Tr[\mathbb{H}\boldsymbol{\sigma}^+\mathbb{H}\boldsymbol{\sigma}^+] \quad (44)$$

$$= Tr[<\mathbb{H}\boldsymbol{\sigma} >_+ <\mathbb{H}\boldsymbol{\sigma} >_+] \quad (45)$$

$$= Tr\left[\left(\sum_{i=1}^2 \lambda_i^+ \boldsymbol{\sigma}_i\right)\left(\sum_{j=1}^2 \lambda_j^+ \boldsymbol{\sigma}_j\right)\right] \quad (46)$$

$$= \sum_i \sum_j \lambda_i^+ \lambda_j^+ Tr[\boldsymbol{\sigma}_i \boldsymbol{\sigma}_j] \quad (47)$$

$$= \sum_{i=1}^2 (\lambda_i^+)^2 \quad (48)$$

First derivative

$$Tr[\boldsymbol{\varepsilon}^e \delta \boldsymbol{\sigma}] = \delta\left(\frac{1}{2} Tr[\mathbf{C}\boldsymbol{\sigma}^+\boldsymbol{\sigma}^+]\right) \quad (49)$$

$$= \sum_{i=1}^2 \lambda_i^+ \delta(\lambda_i^+) \quad (50)$$

$$= \sum_i \lambda_i^+ h(\lambda_i) Tr[\boldsymbol{\sigma}_i \mathbb{H} \delta \boldsymbol{\sigma}] \quad (51)$$

$$= \sum_i \lambda_i^+ Tr[\boldsymbol{\sigma}_i \mathbb{H} \delta \boldsymbol{\sigma}] \quad (52)$$

$$= Tr\left[\left(\sum_i \lambda_i^+ \boldsymbol{\sigma}_i\right) \mathbb{H} \delta \boldsymbol{\sigma}\right] \quad (53)$$

$$= Tr[\mathbb{H} \mathbb{H}^{-1} \left(\sum_{i=1}^2 \lambda_i^+ \boldsymbol{\sigma}_i\right) \mathbb{H} \delta \boldsymbol{\sigma}] \quad (54)$$

$$= Tr[\mathbb{H} \boldsymbol{\sigma}^+ \mathbb{H} \delta \boldsymbol{\sigma}] \quad (55)$$

$$Tr[\boldsymbol{\varepsilon}^e \delta \boldsymbol{\sigma}] = Tr[\mathbf{C}\boldsymbol{\sigma}^+ \delta \boldsymbol{\sigma}] \quad (56)$$

Second derivative

$$Tr\left[\frac{\partial \boldsymbol{\varepsilon}^e}{\partial \boldsymbol{\sigma}} d\boldsymbol{\sigma} \delta \boldsymbol{\sigma}\right] = d(Tr[\mathbf{C}\boldsymbol{\sigma}^+ \delta \boldsymbol{\sigma}]) \quad (57)$$

$$= \sum_{i=1}^2 d(\lambda_i^+) \delta(\lambda_i^+) \quad (58)$$

$$= \sum_{i=1}^2 h(\lambda_i) Tr[\boldsymbol{\sigma}_i \mathbb{H} d\boldsymbol{\sigma}] h(\lambda_i) Tr[\boldsymbol{\sigma}_i \mathbb{H} \delta \boldsymbol{\sigma}] \quad (59)$$

Now, introducing $\boldsymbol{\sigma}_3 = \frac{\sqrt{2}}{2} (T_1 T_2^T + T_2 T_1^T)$, we have the property (due to equations 39 and 43):

$$Tr[\boldsymbol{\sigma}_3 \mathbb{H} d\boldsymbol{\sigma}] = 0 \quad (60)$$

This gives:

$$Tr\left[\frac{\partial \varepsilon^e}{\partial \boldsymbol{\sigma}} d\boldsymbol{\sigma} \delta \boldsymbol{\sigma}\right] = \sum_{i=1}^3 h(\lambda_i) Tr[\boldsymbol{\sigma}_i \mathbb{H} d\boldsymbol{\sigma}] Tr[\boldsymbol{\sigma}_i \mathbb{H} \delta \boldsymbol{\sigma}] \quad (61)$$

$$= Tr\left[\left(\sum_i h(\lambda_i) \mathbb{H} \boldsymbol{\sigma}_i \otimes \boldsymbol{\sigma}_i \mathbb{H}\right) d\boldsymbol{\sigma} \delta \boldsymbol{\sigma}\right] \quad (62)$$

$$Tr\left[\frac{\partial \varepsilon^e}{\partial \boldsymbol{\sigma}} d\boldsymbol{\sigma} \delta \boldsymbol{\sigma}\right] = Tr\left[H \left(\sum_{i=1}^3 h(\lambda_i) \boldsymbol{\sigma}_i \otimes \boldsymbol{\sigma}_i\right) \mathbb{H} d\boldsymbol{\sigma} \delta \boldsymbol{\sigma}\right] \quad (63)$$

Thus: $\frac{\partial \varepsilon^e}{\partial \boldsymbol{\sigma}} = \mathbb{H}(\sum_{i=1}^3 h(\lambda_i) \boldsymbol{\sigma}_i \otimes \boldsymbol{\sigma}_i) \mathbb{H}$. The sum from 1 to 2 doesn't give the good operator but the good trace.

Using the Voigt notation:

$$\frac{\partial \hat{\varepsilon}^e}{\partial \boldsymbol{\sigma}} = \hat{H} \left(\sum_{i=1}^3 h(\lambda_i) \hat{\sigma}_i \hat{\sigma}_i^T\right) \hat{H} \quad (64)$$

Note that if all eigenvalues λ_i are positive (which is not the case if shear appears), we get:

$$d\hat{\boldsymbol{\sigma}}^T \frac{\partial \hat{\varepsilon}^e}{\partial \boldsymbol{\sigma}} \delta \hat{\boldsymbol{\sigma}} = d\hat{\boldsymbol{\sigma}}^T \hat{H} \left(\sum_{i=1}^3 \hat{\sigma}_i \hat{\sigma}_i^T\right) \hat{H} \delta \hat{\boldsymbol{\sigma}} = d\hat{\boldsymbol{\sigma}}^T \hat{H} \hat{H} \delta \hat{\boldsymbol{\sigma}} = d\hat{\boldsymbol{\sigma}}^T \hat{C} \delta \hat{\boldsymbol{\sigma}} \quad (65)$$

the third term of the sum is important to get the identity operator.

B ERROR SIMPLIFICATION

First, note that the modes C_i are supposed to be orthogonal such as $Tr[C_i C_j] = \delta_{ij}$ (δ is the Kronecker symbol). Thus d_i is the projection of $\frac{\partial \varepsilon^e}{\partial \boldsymbol{\sigma}} - \mathbb{C}_0$ on C_i . The error is based on:

$$Tr[\mathbb{C}_{err} \mathbb{C}_{err}] = Tr\left[\left(\sum_i d_i C_i - \frac{\partial \varepsilon^e}{\partial \boldsymbol{\sigma}} - \mathbb{C}_0\right) \left(\sum_j d_j C_j - \frac{\partial \varepsilon^e}{\partial \boldsymbol{\sigma}} - \mathbb{C}_0\right)\right] \quad (66)$$

$$= Tr\left[\left(\frac{\partial \varepsilon^e}{\partial \boldsymbol{\sigma}} + \mathbb{C}_0\right) \left(\frac{\partial \varepsilon^e}{\partial \boldsymbol{\sigma}} + \mathbb{C}_0\right)\right] - 2 \sum_i Tr[d_i C_i \left(\frac{\partial \varepsilon^e}{\partial \boldsymbol{\sigma}} + \mathbb{C}_0\right)] \quad (67)$$

$$+ \sum_{i,j} d_i d_j Tr[C_i C_j] \quad (68)$$

$$= Tr\left[\left(\frac{\partial \varepsilon^e}{\partial \boldsymbol{\sigma}} + \mathbb{C}_0\right) \left(\frac{\partial \varepsilon^e}{\partial \boldsymbol{\sigma}} + \mathbb{C}_0\right)\right] - \sum_i d_i d_i \quad (69)$$

The first term is constant and thus will disappear from the minimization.

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