On the Numerical Modelling of the Cooling Down Process of a SiC Thin Film using a Variable Time-Step Feedback Damping Algorithm

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Abstract: The numerical modelling of the cooling down process of a SiC thin film in an Al substrate is performed using a mathematical model that, in the presence of a variable time step algorithm and a smooth evolution of a state variable, increases the performance of the numerical process, forces the convergence of the numerical solution and, consequently, improves the overall quality of the results. This model corresponds to the generalisation, from a constant step process to a variable step one, of the numerical feedback damping algorithm, previously proposed by the authors. This algorithm is based on the mathematical adjustment of the evolution of a given state variable, which exhibits oscillatory numerical instabilities. The algorithm is implemented and tested with a non-linear finite element example, using a thermoelastic-viscoplastic constitutive model. In order to evaluate the performance of the algorithm, some results, obtained with and without the application of both the constant step and the variable step optimisation algorithms, are presented and thoroughly compared. The variable step numerical damper algorithm proves to be very efficient, allowing a significant reduction of the total number of time steps of the numerical simulation of the cooling down process of a SiC thin film in an Al substrate.

Keywords: Thin Film, Numerical Damping, Variable Time-Step, Incremental Process, Finite Element Method.

1 Introduction

Nowadays, a large number of finite element simulation processes involve the use of highly non-linear algorithms, constitutive models and formulations. This is the case, for example, of the modelling of the cooling down process of a SiC thin film in an Al substrate.

Non-linear formulations inevitably lead to the implementation of incremental algorithms with generic time steps $[t_n, t_n + \Delta t]$ and, consequently, often complex time integration procedures. Thus, the need for efficient and low-cost variable time step optimisation algorithms is ever more needed.

Many algorithms for variable time-step optimisation, adequate for non-linear behaviour models, can be implemented with automatic formulations that anticipate the evolution of the constitutive model parameters and correct the time step in order to avoid both divergence and withdrawal from the constitutive behaviour. This constitutive evolution is often highly unstable, which results in oscillatory numerical instabilities.

In this context, the authors propose, in the present work, a variable-time step generalisation of a numerical feedback damping algorithm previously proposed by themselves [1]. This algorithm consisted in a numerical stabilisation method, based on an analogy with the dynamic response of a classic vibratory system.

The proposed method relies on (i) the mathematical treatment of the evolution of a chosen internal state variable – the control variable – and (ii) the use of an automatic time-step optimisation algorithm [2]. The simultaneous consideration of these optimisation methods results in the so-called variable time-step numerical feedback damping algorithm.

This algorithm, which is summarily presented, was implemented in a non-linear finite element code and validated by the numerical modelling of the cooling down process of a SiC thin film in an Al substrate, considering a thermoelastic-viscoplastic constitutive model [2-5].

2 Modelling

2.1 Feedback damping algorithm

In the feedback damping algorithm, it is assumed assume that, at each Gauss integration point, the numerical results of a non-linear finite element analysis (FEA) can reflect the behaviour of a virtual vibratory system – the numerical code [1]. Therefore, the numerical damping algorithm consists on the replacement, for every Gauss integration point (IP), of some transformation function Θ of a given state variable $\Psi(t)$, by its arithmetic average $\overline{\alpha}(\Theta)$ in the interval $[t_k, t_k+\Delta t]$, *i.e.*,

$$n \in N, \forall \text{IP}: \quad \Theta\left[\Psi\left(t_k+\Delta t\right)\right] \doteq \overline{\alpha}(\Theta) = \frac{\Theta\left[\Psi\left(t_k+\Delta t\right)\right]+\Theta\left[\Psi\left(t_k\right)\right]}{2}. \tag{1}$$

Note that if $\Theta[\Psi(t)] = \Psi(t)$, *i.e.* Θ is the identity transformation, then

$$\Psi\left(t_k+\Delta t\right) \doteq \overline{\alpha}(\Psi) = \frac{\Psi\left(t_k+\Delta t\right)+\Psi\left(t_k\right)}{2}. \tag{2}$$

The value of state variable $\Psi(t_k+\Delta t)$ is therefore replaced by its arithmetic average $\overline{\alpha}(\Psi)$ along the interval $[t_k, t_k+\Delta t]$. On the other hand, if we have $\Theta[\Psi(t)] = \ln[\Psi(t)]$ with $\Psi(t) > 0 \ \forall t$, *i.e.* Θ is the logarithmic transformation, then

$$\ln\left[\Psi\left(t_k+\Delta t\right)\right] = \frac{\ln\left[\Psi\left(t_k+\Delta t\right)\right]+\ln\left[\Psi\left(t_k\right)\right]}{2}, \tag{3}$$

which means that

$$\Psi\left(t_k+\Delta t\right) \doteq \overline{\gamma}(\Psi) = \sqrt{\Psi\left(t_k+\Delta t\right)\times\Psi\left(t_k\right)}. \tag{4}$$

In this case, the value of state variable $\Psi(t_k+\Delta t)$ is therefore replaced by its geometric average $\overline{\gamma}(\Psi)$ along the interval $[t_k, t_k+\Delta t]$.

The background of this algorithm is related to the concept of feedback or to the closed-loop method of Discrete-Time Control Systems [6]. In fact, if the constitutive model (CM) of the finite element code is seen as an ‘‘open-loop system’’, with the implementation of the damping algorithm the CM becomes a sort of ‘‘closed-loop system’’, due to the fact of the previous value of the internal state variable, at instant t_k, being fed back, along with its actual value, to the constitutive model at instant $t_k+\Delta t$ [1].

Nevertheless, it should be noted that the background of the presented algorithm differs substantially from those related to energy decaying schemes [7-9], which attempt to develop robust algorithms for integrating time semidiscrete equations associated with stiff non-linear finite element problems. Since this algorithm is only defined for constant time-step increments Δt, an automatic time-step algorithm must also be considered [2].

2.2 Automatic time-step algorithm

The automatic time-step algorithm is based on a measure of the rate of change of the plastic flow rate tensor [2]. This algorithm uses two step reduction criteria: (i) a criterion based on a scalar control parameter that represents the maximum absolute value, over all the Gauss integration points, of the difference between the equivalent plastic strain rate $\dot{\bar{\varepsilon}}^{\text{p}}$ at the end and beginning of the current increment, multiplied by the size of the time increment itself; (ii) a criterion based on the determination of the maximum value of the increment of the equivalent plastic strain over all the integration points of the structure.

A time-step reduction factor r is calculated after the determination of these two optimisation parameters by combining those two criteria. The time increment size is then updated according to

$$\Delta t_{\text{new}} \leftarrow \frac{r_{\text{cut}}}{r}\Delta t_{\text{old}} \quad \text{or} \quad \Delta t_{\text{new}} \leftarrow r_{\text{enl}}\Delta t_{\text{old}}, \tag{5}$$

whether $r > 1$, leading to a reduction of the time-step size, or $r < 1$, leading to an increase of the time-step size, respectively. r_{cut} is an optimisation reduction factor. The enlargement factor, $r_{\text{enl}} \in [1.1; 2.5]$, can be calculated dynamically for each time-step using

$$r_{\text{enl}} = 2.5 - 1.4\left\{\frac{\exp\left(Fc\,\dfrac{r-0.2}{0.6}\right)-1}{\exp(Fc)-1}\right\}, \tag{6}$$

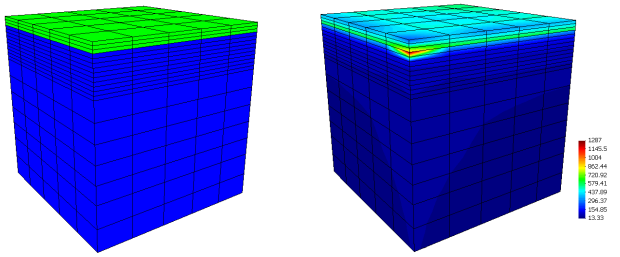
where F_c is a correction factor defining the shape of the optimisation profile [2].

2.3 Numerical modelling

In order to test the optimisation algorithms described in the previous paragraphs, the authors deliberately chose a numerical example that uses a highly non-linear constitutive model. This example is the nume-

rical simulation of cooling down process of SiC thin film in an Al substrate. To solve this example, a set of two constitutive models is used to describe the micromechanical behaviour of the two constituent materials – SiC thin film and Al substrate. These models are thoroughly described, for instance, by Anand [3] and Teixeira-Dias and Menezes [2,4]. The constitutive model for the reinforcement is a classical thermoelastic model [5]. For the metallic substrate, one assumes a rate-dependent, *i.e.* visco-plastic, behaviour. The numerical integration of the constitutive models is made with a forward gradient algorithm, in the form initially proposed by Peirce *et al.* [10] and afterwards developed by Anand *et al.* [11], Lush *et al.* [12], Teodosiu and Menezes [13] and Teixeira-Dias and Menezes [2].

The cooling down process of a SiC thin film in an Al substrate is simulated by finite elements analyses. Initial and final process temperatures are T_i = 933K and T_f = 293K, respectively, and the cooling rate is $\dot{T} = -100\text{Ks}^{-1}$. Numerical simulations are performed using a representative three-dimensional unit cell, discretised in hexahedral three-dimensional finite elements with eight nodes and eight Gauss integration points. Its finite element mesh is shown in Fig. 1(a). In order to avoid the development of locking effects the volumetric part of the displacement gradient is interpolated with a reduced selective scheme [14,15]. The specified boundary conditions were such that coordinate planes *Oxy*, *Oxz* and *Oyz* correspond to planes of symmetry. Fig. 1(b) shows the distribution of the von Mises stress.



(a) (b)

Fig. 1 – Finite element mesh and distribution of the von Mises stress of the representative three-dimensional unit cell.

Note that, as expected, during the cooling down process, the gradient of equivalent stresses tends to be higher near the film-substrate interface, mainly in the external edges' interface. This fact is mainly due to the discontinuity in material properties and the mismatch between the thermal expansion coefficients of the film and the substrate materials.

3 Results and Discussion

3.1 Constant step-time results

The accurate reference solution, *i.e.* the solution without numerical instabilities, was obtained using a very small constant time increment, Δt = 3 ms, which corresponds to a temperature decrement $\Delta T = -0.3$K, and a forward gradient time integration weighting factor equal to 0.25. The latter parameter controls the estimation of the plastic strain rate increment in the forward gradient integration procedure [2]. It should be noted that, since the cooling rate is considered to be constant, the results can be analysed in terms of temperature, instead of time, increments. In this simulation, 2131 temperature constant steps were needed. The accurate equivalent plastic strain rate $\dot{\bar{\varepsilon}}^p$ (EPSR) – the control variable – evolution with the temperature T is presented in Fig. 2. All the presented numerical results were obtained on a specific integration point located in the substrate material, but close to the film–substrate interface.

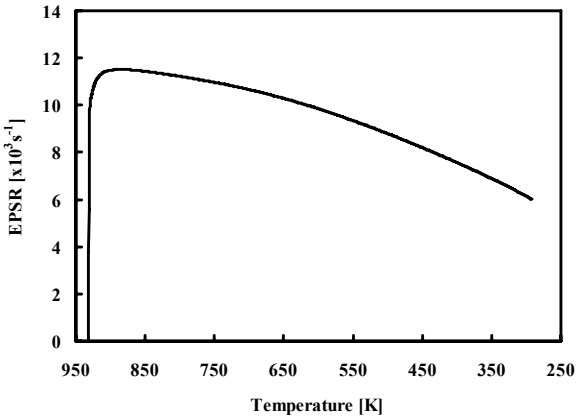


Fig. 2 – Accurate evolution of the equivalent plastic strain rate (EPSR) with temperature, for $\Delta T = -0.3$K (2131 constant steps).

Several numerical simulations were performed considering larger time decrements. Fig. 3 presents the evolution of the EPSR with temperature for $\Delta T = -1.0$K, denominated Signal 1.0, and, for comparison purposes, the accurate results. In this case, 640 steps were needed, but numerical instabilities emerged. This fact can be explained by the conditional stability of the semi-implicit integration method: if the time step is small enough, stability is reached; otherwise instabilities (oscillations) will emerge. Therefore, non-damped oscillations vanish as the time step size is reduced to be sufficiently small to stabilise the semi-implicit integration method and, consequently, lead to a non-oscillatory numerical solution.

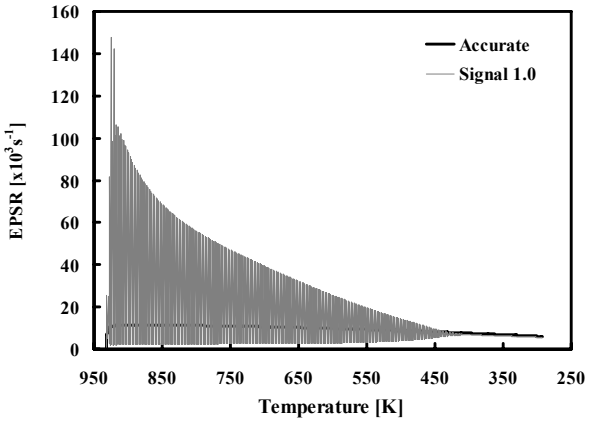


Fig. 3 – Evolution of the equivalent plastic strain rate (EPSR) with temperature, for $\Delta T = -1.0$K (640 constant steps).

As illustrated in Fig. 4, the consideration of the logarithmic transformation of the equivalent plastic strain rate leads to a symmetric evolution of these results about the accurate ones. Since the main objective of the numerical damping algorithm described in Section 2.1 is to reach numerical dynamic stability, it forces the replacement of the actual numerical value, or its transformation, by averaging itself with its predecessor. This methodology refrains the unstable tendencies and, for oscillating numerical signals, leads to the desired approximation to the optimal – equilibrium position – results [1]. These facts suggest that $\Psi(t)$ and Θ should be considered as the equivalent plastic strain rate, $\dot{\bar{\varepsilon}}^{\mathrm{p}}$, and $\ln \dot{\bar{\varepsilon}}^{\mathrm{p}}$, respectively, *i.e.* Θ as the logarithmic function. The importance of the logarithmic Θ resides in the fact that symmetry of a non-damped numerical signal eliminates spurious factors that may distort the analysis of the damped results, since the signal does not possess average value deviation.

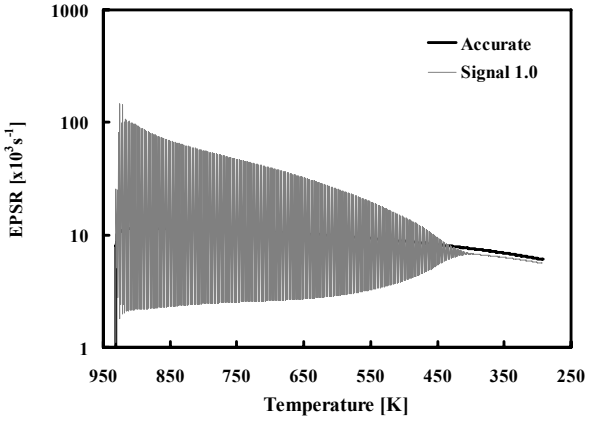


Fig. 4 – Logarithmic evolution of the equivalent plastic strain rate (EPSR) with temperature, for $\Delta T = -1.0$K (640 constant steps).

It should be emphasised that, although a symmetrising transformation leads to better convergence results, in practice, since this transformation function is usually *a priori* unknown, the damping methodology may be implemented considering the identity transformation, *i.e.* the arithmetic mean of the control variable, as a consistent methodology of feedback damping. The main reason for the considering the logarithmic transformation in the present work was the fact that this transformation for the equivalent plastic strain rate led to a symmetric evolution of these results about the accurate ones. Moreover, these considerations do not invalidate the general use of the identity transformation. In reality, the symmetrising transformation may be thought as the upper bound of the algorithm efficiency and not as a *conditio sine qua non* for its systematic implementation [1].

The application of the logarithmic transformation in the feedback algorithm, also denominated γ-method [1], leads to a equivalent plastic strain rate evolution that presents an initial damped vibratory behaviour, as can be observed in Fig. 5. This is similar to what occurs in the dynamic mechanical behaviour of some underdamped vibratory systems.

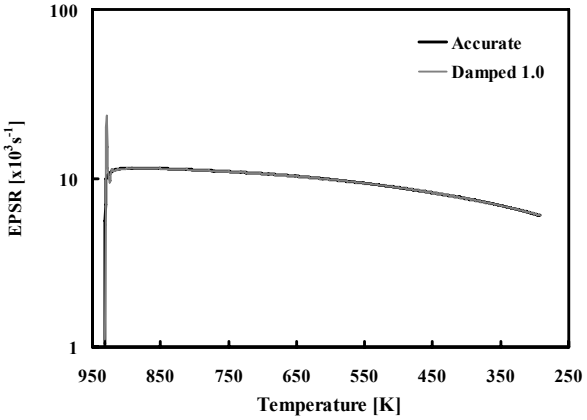


Fig. 5 – Logarithmic evolution of γ-damped equivalent plastic strain rate (EPSR) with temperature, for $\Delta T = -1.0$K (640 constant steps).

In order to observe the non-initial application of this algorithm, a temperature $T_{\mathrm{d}} = 633$K was chosen for the beginning of damping effect. Fig. 6 illustrates the logarithmic evolution of the γ-damped equivalent plastic strain rate with temperature for this specific situation. It can be observed that damping effect becomes more pronounced due to its sudden application, although some initial deviation of the non-initially γ-damped results can be observed in relation to the accurate ones.

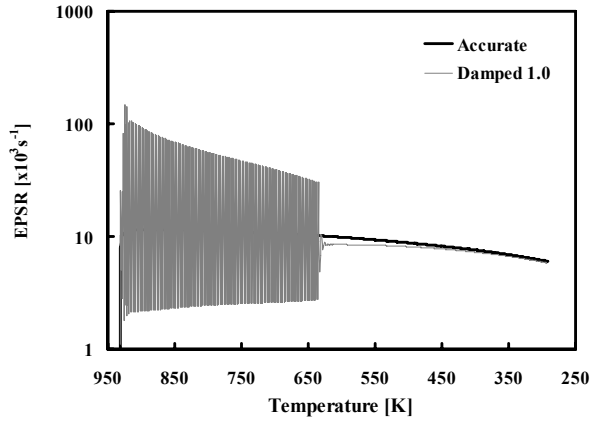


Fig. 6 – Logarithmic evolution of the non-initially γ-damped equivalent plastic strain rate (EPSR) with temperature, for $\Delta T = -1.0$K and $T_d = 633$K (640 constant steps).

3.2 Automatic time-step solution

Although the application of the automatic time-step algorithm results in less necessary steps, it induces, as shown in Fig. 7, stronger numerical instabilities. This may be justified by the fact of the non-damped results present a vibratory nature for decrements larger than $\Delta T = -0.3$K, as referred in Section 3.1.

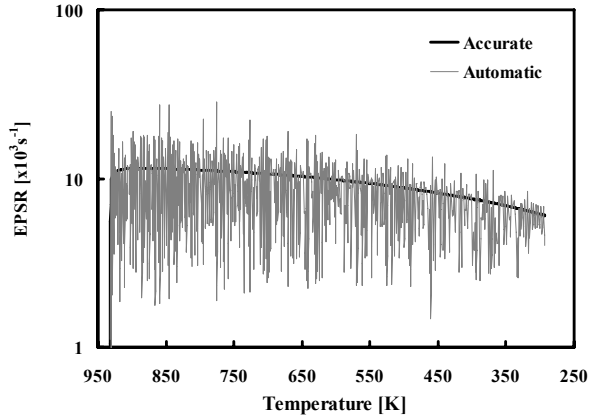


Fig. 7 – Logarithmic evolution of the automatic-step damped equivalent plastic strain rate (EPSR) with temperature (873 variable steps).

In this context, the combination of the γ-damping and the automatic time-step algorithms seems to be the natural way to force the stability of numerical results when large decrements are used.

3.3 Variable time-step damped results

The results of the application of the hybrid variable time-step algorithm are presented in Fig. 8.

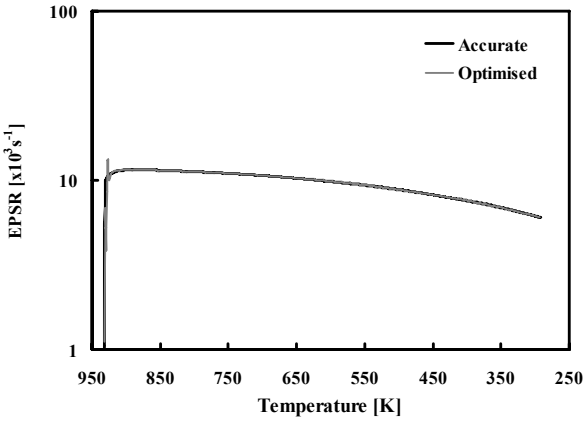


Fig. 8 – Logarithmic evolution of the optimised equivalent plastic strain rate (EPSR) with temperature, for $\Delta T = -1.0$K and $T_d = 633$K (203 variable steps).

Only 203 variable steps were needed to obtain these results, which corresponds to 68.3% and 90.5% reductions in the necessary steps of the γ-damped and the accurate results, respectively. It can then be concluded that this damping algorithm allows the execution of simulation processes using larger time steps, thus saving CPU time, and increasing the precision of the numerical results, proving to be very efficient and appropriate when predicting non-linear thermomechanical behaviour of a SiC thin film in an Al substrate.

4 Conclusions

A numerical variable-time step feedback damping algorithm, applicable to the finite element simulation of non-linear behaviour of materials was presented.

This algorithm was applied and tested with a non-linear finite element example, using a rate dependent constitutive model, in order to evaluate its capabilities. The set of numerical validation tests consisted on the simulation of the cooling down process of a SiC thin film in an Al substrate.

An accurate solution, *i.e.* without numerical instabilities, was obtained for $\Delta T = -0.3$K, corresponding to 2131 computational constant steps.

For $\Delta T = -1.0$K, numerical instabilities emerged and 640 steps were needed.

Therefore, two distinct transformation functions were defined: the identity and the logarithmic functions. Nevertheless, the logarithmic function was used, since it symmetrised the evolution of the state variable. The application of this methodology

refrained the dispersion of the oscillating numerical signals, but required the use of constant steps.

On the other hand, the application of the automatic time-step algorithm resulted in fewer steps, but induced stronger numerical instabilities.

Finally, the use of the hybrid numerical damper algorithm allowed 68.3% and 90.5% reductions in the necessary steps on the γ-damped and the accurate results, respectively. Therefore, it allowed the execution of simulation processes using larger time steps, thus saving CPU time, and eliminating numerical instabilities.

It proved to be very efficient and appropriate when predicting non-linear thermo-mechanical behaviour of a SiC thin film in an Al substrate.

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