AN EFFICIENT, NON-REGULARIZED SOLUTION ALGORITHM FOR A FINITE STRAIN SHAPE MEMORY ALLOY CONSTITUTIVE MODEL

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ABSTRACT

In this paper we investigate a three-dimensional finite-strain phenomenological constitutive model and propose an efficient solution algorithm by properly defining the variables and by avoiding extensively-used regularization schemes which increase the solution time. We define a nucleation-completion criterion and modify the regularized solution algorithm. Implementation of the proposed integration algorithm within a user-defined subroutine UMAT in the commercial nonlinear finite element software ABAQUS has made possible the solution of boundary value problems. The obtained results show the efficiency of the proposed solution algorithm and confirm the improved efficiency (in terms of solution CPU time) when a nucleation-completion criterion is used instead of regularization schemes.

INTRODUCTION

Shape memory alloys (SMAs) are well-known materials exhibiting special properties, known as super-elasticity or pseudo-elasticity (PE), one-way and two-way shape memory effects (SME) [1, 2], suitable for industrial applications. For example, nowadays pseudo-elastic Nitinol is a common and well-known engineering material in the medical industry [3, 4]. The origin of SMA features is a reversible thermo-elastic martensitic phase transformation between a high symmetry, austenitic phase and a low symmetry, martensitic phase. Austenite is a solid phase, usually characterized by a body-centered cubic crystallographic structure, which transforms into martensite by means of a lattice shearing mechanism. When the transformation is driven by a temperature decrease, martensite variants compensate each other, resulting in no macroscopic deformation. However, when the transformation is driven by the application of a load, specific martensite variants, favorable to the applied stress, are preferentially formed, exhibiting a macroscopic shape change in the direction of the applied stress. Upon unloading or heating, this shape change disappears through the reversible conversion of the martensite variants into the parent phase [1, 5].

For a stress-free SMA material, four characteristic temperatures can be identified, defined as the starting and finishing temperatures during forward transformation (austenite to martensite),
\( M_s \) and \( M_f \), as well as the starting and finishing temperatures during reverse transformation, \( A_s \) and \( A_f \). Accordingly, in a stress-free condition, at a temperature above \( A_f \), only the austenitic phase is stable, while at a temperature below \( M_f \), only the martensitic phase is stable. On the other hand, applying a stress at a temperature above \( A_f \), SMAs exhibit pseudo-elastic behavior with a full recovery of inelastic strain upon unloading, while at a temperature below \( M_s \), the material presents the shape memory effect with permanent inelastic strains upon unloading which may be recovered by heating.

The majority of the current 3D macroscopic constitutive models of SMAs has been developed in the pseudo-elastic range and small deformation regime [6–12]. The finite deformation SMA constitutive models available in the literature have been mainly developed by extending small strain constitutive models [13–19]. In the present work we focus on a phenomenological finite-strain SMA constitutive model extensively studied in references [17,20,21] and we improve it by introducing well-defined, non-singular and continuous variables. Moreover, we present the modified solution algorithm by defining a nucleation-completion condition.

### THE FINITE STRAIN SMA CONSTITUTIVE MODEL

Based on a multiplicative decomposition of the deformation gradient, a thermodynamically-consistent finite strain constitutive model has been presented in [17,21]. The model is however singular and a regularized form of the variable has been used to avoid singularity in the solution algorithm. In the following, we briefly review the constitutive model and propose an improved definition to remove the singularity without need to use any kind of regularization. We refer to [22] for more details.

Considering a deformable body, we denote with \( F \) the deformation gradient and with \( J \) its determinant, supposed to be positive. The tensor \( F \) can be uniquely decomposed as:

\[
F = RU = VR
\]

where \( U \) and \( V \) are the right and left stretch tensors, respectively, both positive definite and symmetric, while \( R \) is a proper orthogonal rotation tensor. The right and left Cauchy-Green deformation tensors are then respectively defined as:

\[
C = F^T F, \quad b = FF^T
\]

and the Green-Lagrange strain tensor, \( E \), reads as:

\[
E = \frac{C - 1}{2}
\]

where \( I \) is the second-order identity tensor.

Following a well-established approach adopted in plasticity [23, 24] and already used for SMAs [13–15, 17, 21], we assume a local multiplicative decomposition of the deformation gradient into an elastic part \( F^e \), defined with respect to an intermediate configuration, and a transformation one \( F^t \), defined with respect to the reference configuration. Accordingly:

\[
F = F^e F^t
\]

We define \( C^e = F^e T F^e \) and \( C^t = F^t T F^t \) as the elastic and the transformation right Cauchy-Green deformation tensors, respectively.

In order to satisfy the principle of material objectivity, the Helmholtz free energy \( \Psi \) has to depend on \( F^e \) only through the elastic right Cauchy-Green deformation tensor; it is moreover assumed to be a function of the transformation right Cauchy-Green deformation tensor and of the temperature, \( T \), in the following form:

\[
\Psi = \Psi(C^e, C^t, T) = \psi(C^e) + \psi(E^t, T)
\]

where \( \psi(C^e) \) is a hyperelastic strain energy function (with this choice, we assume that martensitic and austenitic phases have the same elastic behaviors) and \( E^t = (C^t - I)/2 \) is the transformation strain. In addition, we assume \( \psi(C^e) \) to be an isotropic function of \( C^e \). We also define \( \psi \) in the following form [8]:

\[
\psi(E^t, T) = \tau_M(T) \|E^t\| + \frac{1}{2} h \|E^t\|^2 + I_{\varepsilon_L}(\|E^t\|) \tag{6}
\]

where \( \tau_M(T) = \beta(T - T_0) \) and \( \beta, T_0 \) and \( h \) are material parameters, while the Maclaurin brackets calculate the positive part of the argument, i.e., \( \langle x \rangle = (x + |x|)/2 \), and the norm operator is defined as \( \|A\| = \sqrt{A : A} \), with \( A : B = A_{ij} B_{ij} \). Moreover, in equation (6) we also use the indicator function \( I_{\varepsilon_L} \) defined as:

\[
I_{\varepsilon_L}(\|E^t\|) = \begin{cases} \text{0} & \text{if } \|E^t\| \leq \varepsilon_L \\ +\infty & \text{otherwise} \end{cases} \tag{7}
\]

in order to impose the constraint on the transformation strain norm (i.e., \( \|E^t\| \leq \varepsilon_L \)). The material parameter \( \varepsilon_L \) is the maximum transformation strain norm in a uniaxial test.

We now use Clausius-Duhem inequality form of the second law of thermodynamics:

\[
S : \frac{1}{2} \dot{C} - (\Psi + \eta \dot{T}) \geq 0 \tag{8}
\]
where \( S \) is the second Piola-Kirchhoff stress tensor and is obtained from the Cauchy stress as:

\[
S = JF^{-1} \sigma F^{-T}
\]

(9)

Substituting (5) into (8) and following standard arguments, we obtain the constitutive model as already presented in [17, 21]

We highlight that the material parameters \( \lambda \) and \( \mu \) are the Lam\`e constants and the positive variable \( \gamma \) results from the indicator function subdifferential.

<table>
<thead>
<tr>
<th>Table 1. Finite-strain SMA constitutive model</th>
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**External variables:** \( C, T \)

**Internal variable:** \( C' \)

**Stress quantities:**

\[
S = 2(\alpha_1 C' + \alpha_2 C' C C^{-1})
\]

\[
Y = CS - C'X
\]

\[
X = hE + (\tau_M + \gamma) N
\]

with

\[
\begin{cases}
\gamma \geq 0 \text{ if } ||E'|| = \varepsilon_L \\
\gamma = 0 \text{ if } ||E'|| < \varepsilon_L
\end{cases}
\]

and

\[
\alpha_1 = \frac{1}{\mu} \left( C : C'^{-1} - 3 \right) - \frac{1}{2}\mu, \quad \alpha_2 = \frac{1}{\mu}
\]

\[
N = \frac{E'}{||E'||} \text{ where } E' = (C' - 1)/2
\]

**Evolution equation:**

\[
\dot{C}' = 2\tilde{\varepsilon} ||Y^D|| C' = \tilde{\varepsilon} A
\]

**Limit function:**

\[
f = ||Y^D|| - R
\]

**Kuhn-Tucker conditions:**

\[
f \leq 0, \quad \tilde{\varepsilon} \geq 0, \quad \tilde{\varepsilon} f = 0
\]

**Proposing a singular-free and continuous definition for \( N \)**

We note that the variable \( N \) is not defined for the case of vanishing transformation strain. Despite some discussions in [20], regularization schemes have extensively been used in the literature to overcome this problem. For example Helm and Haupt [25] propose the following regularization scheme also used in [7, 15, 16, 21]:

\[
||E'|| = \sqrt{||E'||^2 + \delta - \delta}
\]

(10)

where \( \delta \) is a user defined parameter (typical value: \( 10^{-7} \)). In Auricchio and Petrini [26] and adopted also in [17, 27], another proposed regularization scheme is as follows:

\[
||E'|| = ||E'|| - \frac{d^{2+1}}{d - 1} (||E'|| + d)^{d-1}
\]

(11)

where \( d \) is again a user defined parameter (typical value: 0.02).

Both regularization schemes (10) and (11) are indeed equivalent, despite they have different forms.

While using a regularization scheme has some advantages in removing the singularity in \( N \) and in giving a smooth transition from austenitic to martensitic phase and vice versa, with a quite simple approach it has however the disadvantage of transforming a large part of the elastic region into a region of nonlinear material response. This has the disadvantage of significantly increased solution time and consequently decreased numerical efficiency, especially for boundary value problems in which a considerable part of the structure remains elastic (as e.g., in stent structures). In the following, motivated by the work by Argghavani et al. [12] in the small-strain regime, we suggest to avoid using a regularized form for \( ||E'|| \) but to deal with the case of vanishing transformation strain through a careful analytical study of the limiting conditions.

We start investigating a condition in which \( E' \) starts to evolve from a zero value (Nucleation), i.e., \( E' = 0 \) while \( d ||E'||/d > 0 \). Substituting \( C' \approx I \) into the evolution equation we conclude \( Y^D \approx (C S_r)^D \). We now consider the evolution equation which yields:

\[
E' = \frac{1}{2} C' = \tilde{\varepsilon} (C S_r)^D \| (C S_r)^D \|
\]

(12)

where \( S_r = 2(\alpha_1 I + \alpha_2 C) \) is the elastic stress obtained from the second Piola-Kirchhoff stress tensor by substituting \( I \) in place of \( C' \). According to (12) the transformation strain, \( E' \), nucleates in the \( (C S_r)^D \) direction.

We now investigate a case when transformation strain vanishes from a nonzero value (Completion), i.e., \( E' = 0 \) (\( C' = I \)) while \( d ||E'||/d < 0 \). Since \( ||E'|| = 0 \), we conclude that adopting any arbitrary direction \( N \) leads to \( E' = 0 \). Following [12] (for a small-strain case), we select the \( (C S_r)^D \) direction which also guarantees continuity. Therefore, we revise the variable \( N \) in the fol-
following form:

$$N = \begin{cases} 
\frac{(CS_e)^D}{\| (CS_e)^D \|} & \text{if } \| E' \| = 0 \\
E' & \text{if } \| E' \| \neq 0 
\end{cases} \quad (13)$$

We note that, according to the above discussion, the tensor $N$ and consequently the tensor $X$ are well-defined, non-singular and continuous.

**TIME-DISCRETE FRAME AND SOLUTION ALGORITHM**

In this section we investigate the numerical solution of the constitutive model summarized in Table 1 while taking into account the improved variable definition (13) and avoiding regularized schemes (10) and (11). The time-discrete form of the evolution equation which conserves the incompressibility condition is obtained through an exponential mapping and is given as follows [15, 16]:

$$-C_n^{-1} + U^{-1} \exp \left( \Delta \tau U^{-1} A U^{-1} \right) U^{-1} = 0 \quad (14)$$

As usual in computational inelasticity problems, we use an elastic predictor-inelastic corrector procedure to solve the time-discrete constitutive model. The algorithm consists of evaluating an elastic trial state, in which the internal variable remains constant, and of verifying the admissibility of the trial function. If the trial state is admissible, the step is elastic; otherwise the step is inelastic and the transformation internal variable has to be updated through integration of the evolution equation.

In order to solve the inelastic step, we use another predictor-corrector scheme, that is, we assume $\gamma = 0$ (i.e., we predict an unsaturated transformation strain case with $\| E' \| \leq \varepsilon_L$) and we solve the following system of nonlinear equations (we refer to this system as PT1 system):

$$\begin{align*}
R^t &= -C_n^{-1} + U^{-1} \exp \left( \Delta \tau U^{-1} A U^{-1} \right) U^{-1} = 0 \\
R^s &= \| Y^D \| - R = 0
\end{align*} \quad (15)$$

If the solution is non-admissible (i.e., $\| E' \|_{PT1} > \varepsilon_L$), we assume $\gamma > 0$ (i.e., we consider a saturated transformation case with $\| E' \| = \varepsilon_L$) and we solve the following system of nonlinear equations (we refer to this system as PT2 system):

$$\begin{align*}
R^t &= -C_n^{-1} + U^{-1} \exp \left( \Delta \tau U^{-1} A U^{-1} \right) U^{-1} = 0 \\
R^s &= \| Y^D \| - R = 0 \\
R^f &= \| E' \| - \varepsilon_L = 0
\end{align*} \quad (16)$$

Solution of equations (15) and (16) is in general approached through a straightforward Newton-Raphson method and it does not reserve special difficulties except for the cases in which the transformation strain vanishes. Accordingly, in the following, we specifically investigate the nucleation ($E' \equiv 0$) and completion ($E' = 0$) cases and construct the solution algorithm.

**Considerations on nucleation-completion condition**

We first investigate the trial value of the limit function in the nucleation case as follows:

$$f^{TR} = \| (CS_e)^D \| - \tau_M(T) - R = \| (CS_e)^D \| - \tau_M(T) - R > 0 \quad (17)$$

where a superscript $TR$ represents the trial value. We may now introduce the following as the *nucleation condition*:

$$\| (CS_e)^D \| > \tau_M(T) + R \quad \text{and} \quad \| E'_n \| = 0 \quad (18)$$

In the solution procedure, when $\| E'_n \| = 0$ we check the nucleation condition and if not satisfied, we assume an elastic behavior.

We remark that, to avoid singularity in local system (15) for the nucleation case, it is necessary to use a nonzero initial transformation strain (initial guess for Newton-Raphson method). Since, we know the initial transformation strain direction, we conclude:

$$C_0 = 1 + 2qN, \quad N = \frac{(CS_e)^D}{\| (CS_e)^D \|} \quad (19)$$

where a subscript $0$ denotes the initial guess. A value of $10^{-4}$ could be an appropriate choice for $q$.

We now focus on the completion case, i.e., $E'_n \neq 0$ but $E' = 0$. To this end, we consider the evolution equation and substitute $C^D = I$ (as it happens for the completion case) to obtain:

$$2\Delta \tau \frac{Y^D}{\| Y^D \|} = \log \left( C_n^{-1} \right) = -\log \left( C_n' \right), \quad Y^D = (CS_e)^D - \tau_M N \quad (20)$$

To study the completion condition, using equation (20) which defines the $Y^D$ direction and considering the limit function definition, we conclude:

$$Y^D = -R \frac{\log \left( C_n' \right)}{\| \log \left( C_n' \right) \|} \quad (21)$$

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Substituting (21) in (20), we obtain:

\[
(CS_e)^D + R \frac{\log(C_n^0)}{\log(C_n^0)} = \tau_M N
\]  

Finally taking the norm of both sides of equation (22), we define the following completion condition:

\[
\left\| (CS_e)^D + R \frac{\log(C_n^0)}{\log(C_n^0)} \right\| \leq \tau_M , \quad \left\| E_n^r \right\| \neq 0 \tag{23}
\]

Therefore, in the solution procedure we also should check the completion condition and if it is satisfied, we simply update the internal variable by setting \( C_t^{0} = 1 \).

Table 2 presents the proposed solution algorithm based on a Nucleation – Completion (NC) scheme.

**Table 2. Solution algorithm using NC condition**

1. compute \( C = F^T F \)
2. compute \( (CS_e)^D \)
3. if \( \left\| (CS_e)^D \right\| < \tau_M + R \) and \( \left\| E_n^r \right\| = 0 \) then
   set \( C_t^{0} = 1 \)
   else
   set \( C_t^{TR} = C_n^0 \) and compute \( f^{TR} \) and trial solution
   if \( f^{TR} < 0 \) then
       Accept the trial solution
   else if (completion condition (23)) then
       set \( C_t^{0} = 1 \)
   else
       if \( \left\| E_n^r \right\| = 0 \) then set \( C_n^0 \) value by (19)
       if \( \left\| E_n^r \right\|_{PT1} < \epsilon_L \) then
           Accept PT1 solution
       else
           solve PT2 system
   end if
end if
**Helical spring**

A helical spring (with a wire diameter of 4mm, a spring external diameter of 24mm, a pitch size of 12mm and with two coils and an initial length of 28mm) is simulated using 9453 quadratic tetrahedron (C3D10) elements and 15764 nodes. An axial force of 1525N is applied to one end while the other is completely fixed. The force is increased from zero to its maximum value and unloaded back to zero. Figure 2 shows the spring initial geometry, the mesh and the deformed shape under the maximum force. After unloading, the spring recovers the original shape as it is expected in the pseudo-elastic regime. Figure 3 shows the force-displacement diagram. It is observed that the spring shape is fully recovered after load removal.

**Crimping of a medical stent**

In this example, the crimping of a pseudo-elastic medical stent is simulated. To this end, a stent with 0.216mm thickness and an initial outer diameter of 6.3mm (Figure 4, top) is crimped to an outer diameter of 1.5mm. Utilizing the ABAQUS/Standard contact module, the contact between catheter and stent is considered in the simulation. A radial displacement is applied to the catheter and then released to reach the initial diameter. In this process, the stent recovers its original shape after unloading. Figure 4 (bottom) shows the stent deformed shape when crimped.

**Comparison of CPU times**

We now compare the CPU times in order to show the efficiency gained by using a nucleation-completion scheme. We remark that we have normalized the CPU times with respect to the CPU times for the case of using regularization (Reg) scheme (10).

Table 3 shows that using the NC scheme decreases the CPU time compared with the Reg scheme. This decrease depends on the problem and for the simulated problems it varies from 11% (spring) to 16% (stent). We remark that, the gained efficiency is also dependent on the temperature and is increased with increasing temperature and vice versa (this fact is due to the longer elastic portion at an higher temperature).

We finally highlight that using the proposed improvement can remarkably decrease the solution time in the simulation of SMA-based devices during design, analysis and optimization processes.

<table>
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<th>Table 3. CPU times comparison</th>
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<td>Example</td>
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<tr>
<td>Spring</td>
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<td>Stent</td>
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**SUMMARY AND CONCLUSION**

In this paper, we discuss an improved constitutive model for a 3D shape memory alloy as well as the corresponding solution algorithm. We introduce a well-defined form for model variables as well as a nucleation-completion scheme to avoid extensively-used regularization schemes. Implementing the proposed integration algorithm within a user-defined subroutine (UMAT) in the commercial nonlinear finite element software ABAQUS, we solve some boundary value problems. Comparing CPU times, we show the gain in efficiency (in the order of 15%) of the proposed time-integration and solution algorithm.
Figure 3. Force-displacement diagram for the SMA spring.

Figure 4. Stent crimping: initial geometry (top), crimped shape (bottom)

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