1D SMA Model (Implicit Integration Scheme)

1 One-dimensional SMA Model

The one-dimensional SMA model is found in [1]. The total strain ε is found using an additive between elastic ε^{el}, thermal expansion ε^{th}, and transformation strain ε^{t} as follows:

$$\varepsilon = \varepsilon^{el} + \varepsilon^{th} + \varepsilon^{t}. \tag{1}$$

The elastic and thermal expansion strains are given by the following formulas:

$$\varepsilon^{el} = E(\xi)^{-1}\sigma, \tag{2}$$

$$\varepsilon^{th} = \alpha(T - T_0), \tag{3}$$

where E is the Young's modulus that depends on the martensitic volume fraction ξ, σ is the uniaxial stress, α is the thermoelastic expansion coefficient, T is the temperature, and T_0 is the initial (reference) temperature. The Young's modulus, dependent on the martensitic volume fraction, is given as follows:

$$E(\xi) = \left[\frac{1}{E^A} + \xi\left(\frac{1}{E^M} - \frac{1}{E^A}\right)\right]^{-1} \tag{4}$$

Substituting Eqs. (2) and (3) into Eq. (1) and solving for the stress, the following is found:

$$\sigma = E(\xi)[\varepsilon - \alpha(T - T_0) - \varepsilon^{t}]. \tag{5}$$

The evolution equation for the transformation strain is related to the evolution of martensitic volume fraction as follows:

$$\dot{\varepsilon}^{t} = \dot{\xi}\Lambda^{t}; \qquad \Lambda^{t} = \begin{cases} H^{cur}(\sigma)\mathrm{sgn}(\sigma); & \dot{\xi} > 0, \\ \varepsilon^{t-r}/\xi^{r}; & \dot{\xi} < 0. \end{cases}, \tag{6}$$

where Λ^{t} is the transformation direction, H^{cur} is the current transformation strain, ε^{t-r} is the transformation strain at transformation reversal, and ξ^{r} is the martensitic volume fraction at transformation reversal. The current transformation strain is given by the following piecewise equation with a constant domain and a decaying exponential function:

$$H^{cur}(\sigma) = \begin{cases} H_{min}; & |\sigma| \le \bar{\sigma}_{crit} \\ H_{min} + (H_{sat} - H_{min})(1 - e^{-k(|\sigma| - \bar{\sigma}_{crit})}); & |\sigma| > \bar{\sigma}_{crit}. \end{cases}. \tag{7}$$

The evolution of the martensitic volume fraction is constrained by the following equations:

$$\Phi^{t} \le 0, \qquad \Phi^{t}\dot{\xi} = 0, \qquad 0 \le \xi \le 1, \tag{8}$$

where the first two represent the Karush-Kuhn-Tucker constraints and the third bounds the martensitic volume fraction, which ranges between 0 (100% austenite) to 1 (100% martensite). The transformation surface has a branched form for forward (austenite to martensite) and reverse (martensite to austenite) transformation:

$$\Phi^t = \begin{cases} \Phi^t_{fwd}, & \dot{\xi} > 0, \\ \Phi^t_{rev}, & \dot{\xi} < 0. \end{cases} \tag{9}$$

The transformation surfaces are the following:

$$\Phi^t_{fwd}(\sigma, T, \xi) = (1-D)|\sigma|H^{cur}(\sigma) + \frac{1}{2}\left(\frac{1}{E^M} - \frac{1}{E^A}\right)\sigma^2 + \rho\Delta s_0 T - \rho\Delta u_0 - f^t_{fwd}(\xi) - Y^t_0, \tag{10}$$

$$\Phi^t_{rev}(\sigma, T, \xi) = -(1+D)\sigma\frac{\varepsilon^{t-r}}{\xi^r} - \frac{1}{2}\left(\frac{1}{E^M} - \frac{1}{E^A}\right)\sigma^2 - \rho\Delta s_0 T + \rho\Delta u_0 + f^t_{rev}(\xi) - Y^t_0. \tag{11}$$

The hardening functions are given as follows:

$$f^t_{fwd}(\xi) = \frac{1}{2}a_1(1 + \xi^{n_1} - (1-\xi)^{n_2}) + a_3, \tag{12}$$

$$f^t_{rev}(\xi) = \frac{1}{2}a_2(1 + \xi^{n_3} - (1-\xi)^{n_4}) - a_3. \tag{13}$$

The parameters defining the transformation surface D, $\rho\Delta s_0$, $\rho\Delta u_0$, Y^t_0, a_1, a_2, and a_3 are calibrated from the SMA phase diagram using the following equations:

$$a_1 = \rho\Delta s_0(M_f - M_s), \tag{14}$$

$$a_2 = \rho\Delta s_0(A_s - A_f), \tag{15}$$

$$a_3 = -\frac{a_1}{4}\left(1 + \frac{1}{n_1+1} - \frac{1}{n_2+1}\right) + \frac{a_2}{4}\left(1 + \frac{1}{n_3+1} - \frac{1}{n_4+1}\right), \tag{16}$$

$$\rho\Delta u_0 = \frac{\rho\Delta s_0}{2}\left(M_s + A_f\right), \tag{17}$$

$$Y^t_0 = \frac{\rho\Delta s_0}{2}(M_s - A_f) - a_3, \tag{18}$$

$$\rho\Delta s_0 = \frac{-2\left(C^M C^A\right)\left[H^{cur}(\sigma) + \sigma\partial_\sigma H^{cur}(\sigma) + \sigma\left(\frac{1}{E^M} - \frac{1}{E^A}\right)\right]}{C^M + C^A}\Big|_{\sigma=\sigma^*} \tag{19}$$

$$D = \frac{\left(C^M - C^A\right)\left[H^{cur}(\sigma) + \sigma\partial_\sigma H^{cur}(\sigma) + \sigma\left(\frac{1}{E^M} - \frac{1}{E^A}\right)\right]}{\left(C^M + C^A\right)\left[H^{cur}(\sigma) + \sigma\partial_\sigma H^{cur}(\sigma)\right]}\Big|_{\sigma=\sigma^*} \tag{20}$$

Where the hardening parameters n_1, n_2, n_3, and n_4 determine the level of smoothness in the transitions between transformation and thermoelastic loading domains and σ^* is the calibration stress for the forward and reverse transformation slopes C^M and C^A. The term $\partial_\sigma H^{cur}(\sigma)$ is defined using the derivative of Eq. (7) with respect to the effective von Mises stress:

$$\partial_\sigma H^{cur}(\sigma) = \begin{cases} 0; & |\sigma| \leq \bar{\sigma}_{crit} \\ k(H_{sat} - H_{min})e^{-k(|\sigma| - \bar{\sigma}_{crit})}\frac{\partial|\sigma|}{\partial\sigma}; & |\sigma| > \bar{\sigma}_{crit}. \end{cases} . \tag{21}$$

Here it is assumed that $\frac{\partial|\sigma|}{\partial\sigma} = 0$ when $\sigma = 0$, since the derivative is undefined at that point:

$$\frac{\partial|\sigma|}{\partial\sigma} = \begin{cases} 1; & \sigma > 0 \\ -1; & \sigma < 0 \\ 0; & \sigma = 0 \end{cases} . \tag{22}$$

2 One-dimensional SMA Model Implementation

In order to discretize Eq. (6) in time, one can use the general trapezoidal rule as follows:

$$\varepsilon^t_{n+1} = \varepsilon^t_n + (\xi_{n+1} - \xi_n)[(1-\beta)\Lambda^t_n + \beta\Lambda^t_{n+1}], \tag{23}$$

where the subscript n represents variables evaluated at the last time t_n and n_1 represents variables to be determined at the next time t_{n+1}. The algorithmic parameter β ranges from 0 to 1 and is often chosen and the held constant during analysis [2, 3]. Here the focus is on the cases where $\beta = 1$ ("Implicit integration scheme").

2.1 Strain-driven, Implicit Integration Scheme

In this implementation, the total strain and the temperature are known during the entire analysis (i.e. they are applied). One example of this type of loading is the displacement controlled loading of an SMA wire under quasi-static conditions (constant temperature).

The numerical implementation of the SMA model of Section 1 requires the solution of stress σ, transformation strain ε^t, and martensite volume fraction ξ at each loading increment.

For this implicit integration scheme, it is required to enforce the condition $\Phi^t \leq 0$ in Eq. (8) by *implicitly* solving for martensitic volume fraction that enforces such a condition given values of stress and temperatures. To do this, an iterative process must be used to find ε^t at each load step. The transformation strain at each iteration k is given by the following equations from [1]:

$$\varepsilon_{n+1}^{t(k+1)} = \varepsilon_n^t + \left(\xi_{n+1}^{(k+1)} - \xi_n\right) \Lambda^t \left(\sigma_{n+1}^{(k+1)}\right) \tag{24}$$

The value is updated through each iteration using:

$$\varepsilon_{n+1}^{t(k+1)} = \varepsilon_{n+1}^{t(k)} + \Delta\varepsilon_{n+1}^{t(k)} \tag{25}$$

A simplification to this integration comes from relaxing the implicit dependence on the transformation direction, which gives the equation for the change in ε at each iteration:

$$\Delta\varepsilon_{n+1}^{t(k)} = \Delta\xi_{n+1}^{(k)} \Lambda^t \left(\sigma_{n+1}^{(k)}\right) \tag{26}$$

The loading increment at each iteration k is defined as:

$$\sigma_{n+1}^{(k)} = E\left(\xi_{n+1}^{(k)}\right)\left[\varepsilon_{n+1} - \varepsilon_{n+1}^{th} - \varepsilon_{n+1}^{t(k)}\right] \tag{27}$$

During each iteration, the total current strain and temperature are held constant:

$$\Delta\varepsilon_{n+1}^{(k)} = 0,\ \ \Delta T_{n+1}^{(k)} = 0 \tag{28}$$

The stress correction at each iteration is defined as:

$$\Delta\sigma_{n+1}^{(k)} = -E_{n+1}^{(k)}\left(\Delta S \sigma_{n+1}^{(k)} + \Lambda_{n+1}^{t(k)}\right)\Delta\xi_{n+1}^{(k)} \tag{29}$$

Where ΔS is defined as:

$$\Delta S = \frac{1}{E^M} - \frac{1}{E^A} \tag{30}$$

Finally, the correction for ξ at each iteration can be found using the derivation found in [1]:

$$\Delta\xi_{n+1}^{(k)} = \frac{-\Phi_{n+1}^{t(k)}}{A^t} \tag{31}$$

where

$$A^t = \partial_\xi \Phi_{n+1}^{t(k)} - \partial_\sigma \Phi_{n+1}^{t(k)} E_{n+1}^{(k)}\left(\Delta S \sigma_{n+1}^{(k)} + \Lambda_{n+1}^{t(k)}\right) \tag{32}$$

This equation requires two partial derivatives, $\partial_\xi \Phi^t$ and $\partial_\xi \Phi^t$. The first of these is calculated different ways depending on the direction of transformation and the sign of the stress. For forward transformations, the following equations are derived from Eq. (10), with $\partial_\sigma H^{cur}(\sigma)$ defined in Eq. (21). When $\sigma = 0$ the derivative of $|\sigma|$ is assumed to be zero since the derivative is undefined at that point:

$$\partial_\sigma \Phi^t_{fwd} = \begin{cases} -\left(1-D\right)H^{cur}\left(\sigma\right) + \left(1-D\right)|\sigma|\partial_\sigma H^{cur}(\sigma) + \left(\frac{1}{E^M} - \frac{1}{E^A}\right)\sigma; & \sigma < 0 \\ \left(1-D\right)H^{cur}\left(\sigma\right) + \left(1-D\right)|\sigma|\partial_\sigma H^{cur}(\sigma) + \left(\frac{1}{E^M} - \frac{1}{E^A}\right)\sigma; & \sigma > 0 \\ 0; & \sigma = 0 \end{cases} . \tag{33}$$

For reverse transformations, the following equation is derived from Eq. (11):

$$\partial_\sigma \Phi^t_{rev} = -(1+D)\frac{\varepsilon^{t-r}}{\xi^r} - \left(\frac{1}{E^M} - \frac{1}{E^A}\right)\sigma \tag{34}$$

Similar steps can be taken to find the partial derivative of transformation surface Φ^t with respect to martensitic volume fraction ξ. These values are dependent on the partial derivative of the hardening function f^t:

$$\begin{aligned} \partial_\xi \Phi^t_{fwd} &= -\partial_\xi f^t_{fwd}(\xi) \\ \partial_\xi \Phi^t_{rev} &= \partial_\xi f^t_{rev}(\xi) \end{aligned} \tag{35}$$

The derivative of this value becomes infinite as the martensitic volume fraction approaches 0 or 1. To approximate this value numerically, the following function is used to define the hardening function during calculation of Φ^t and $\partial_\xi \Phi^t$, where the constant $\delta << \xi$ is used to address the difficulties in computation:

$$f^t_{fwd} = \frac{1}{2}a_1\left[1 + \left(\frac{\xi^{\frac{1}{n_1}}}{(\xi+\delta)^{\frac{1}{n_1}-1}}\right)^{n_1} - \left(\frac{(1-\xi)^{\frac{1}{n_2}}}{(1-\xi+\delta)^{\frac{1}{n_2}}-1}\right)^{n_2}\right] + a_3 \tag{36}$$

$$f^t_{rev} = \frac{1}{2}a_2\left[1 + \left(\frac{\xi^{\frac{1}{n_3}}}{(\xi+\delta)^{\frac{1}{n_3}}-1}\right)^{n_3} - \left(\frac{(1-\xi)^{\frac{1}{n_4}}}{(1-\xi+\delta)^{\frac{1}{n_4}}-1}\right)^{n_4}\right] - a_3 \tag{37}$$

Using the inequalities $0 < n_i \leq 1,\ i = 1, ..., 4,\ \delta > 0$, and $0 \leq \xi \leq 1$, the expressions for $\partial_\xi f^t_{fwd}$ and $\partial_\xi f^t_{rev}$ are simplified as follows:

$$\begin{aligned} \partial_\xi f^t_{fwd}(\xi) = \;& \frac{1}{2}\Big(-\left(1-\xi+\delta\right)^{n_2-2} n_2\xi + \xi\left(\xi+\delta\right)^{n_1-2} n_1 + \left(1-\xi+\delta\right)^{n_2-2}\delta \\ & + \left(1-\xi+\delta\right)^{n_2-2} n_2 + \left(\xi+\delta\right)^{n_1-2}\delta\Big)\, a_1 \end{aligned} \tag{38}$$

$$\begin{aligned} \partial_\xi f^t_{rev}(\xi) = \;& \frac{1}{2}\Big(-\left(1-\xi+\delta\right)^{n_4-2} n_4\xi + \xi\left(\xi+\delta\right)^{n_3-2} n_3 + \left(1-\xi+\delta\right)^{n_4-2}\delta \\ & + \left(1-\xi+\delta\right)^{n_4-2} n_4 + \left(\xi+\delta\right)^{n_3-2}\delta\Big)\, a_2 \end{aligned} \tag{39}$$

Finally, the inelastic strain ε^t at each iteration can be calculated using the values attained:

$$\varepsilon_{n+1}^{t(k+1)} = \varepsilon_{n+1}^{t(k)} + \Delta\xi_{n+1}^{(k)}\Lambda_{n+1}^{t(k)} \tag{40}$$

The updated stress can then be found using the transformation strain and updated elastic stiffness. This stress value can be used in to calculate the updated transformation function for each iteration. This method of iterating values continues until $\Phi_{n+1}^{t(k+1)}$ is smaller than a chosen tolerance or $\xi_{n+1}^{(k+1)}$ reaches a bound of 0 or 1. Table 1 shows the algorithm for this implementation.

References

[1] D. Lagoudas, D. Hartl, Y. Chemisky, L. Machado, and P. Popov. Constitutive model for the numerical analysis of phase transformation in polycrystalline shape memory alloys. *International Journal of Plasticity*, 32:155–183, 2012.

[2] M.A. Qidwai and D.C. Lagoudas. Numerical implementation of a shape memory alloy thermomechanical constitutive model using return mapping algorithms. *International Journal for Numerical Methods in Engineering*, 47(6):1123–1168, 2000.

[3] G. Scalet, F. Auricchio, and D.J. Hartl. Efficiency and effectiveness of implicit and explicit approaches for the analysis of shape-memory alloy bodies. *Journal of Intelligent Material Systems and Structures*, page 1045389X15592483, 2015.

Table 1: SMA 1D implementation for implicit forward Euler integration scheme. The goal is to solve for σ_{n+1}, ξ_{n+1}, and ε^t_{n+1} given values of strain ε_{n+1} and temperature T_{n+1} using a iterative process at each loading increment.

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(1) Initialize: Let $\xi^{(0)}_{n+1} = \xi_n$, $\varepsilon^{t(0)}_{n+1} = \varepsilon^t_n$, $E^{(0)}_{n+1} = E_n$, $\xi^r_{n+1} = \xi^r_n$, $\varepsilon^{t-r}_{n+1} = \varepsilon^{t-r}_n$

(2) Elastic prediction

- (a) $\sigma^{(0)}_{n+1} = E^{(0)}_{n+1}[\varepsilon_{n+1} - \alpha(T_{n+1} - T_0) - \varepsilon^{t(0)}_{n+1}]$
- (b) Evaluate $\Phi^{t(0)}_{fwd,}$
- (c) Evaluate $\Phi^{t(0)}_{rev}$
- (d) `IF` $\Phi^{t(0)}_{fwd} > 0$ then `chck = 1`
- (e) `ELSE IF` $\Phi^{t(0)}_{rev} > 0$ then `chck = 2`
- (f) `ELSE chck` $= 0$ `EXIT` (Elastic Response)

(3) Transformation correction:

- (a) `IF chck` $= 1$ then correct for forward transformation
- (b) Calculate $\Delta\xi^k_{n+1}$ from Eq. (31)
- (c) Update $\xi^{(k+1)}_{n+1} = \xi^k_{n+1} + \Delta\xi^k_{n+1}$
- (d) Update $\varepsilon^{t(k+1)}_{n+1}$ using Eq. (40)
- (e) Update $E^{(k+1)}_{n+1}$ using Eq. (4)
- (f) Update $\sigma^{(k+1)}_{n+1}$ using Eq. (5)
- (g) Update $\varepsilon^{t-r}_{n+1} = \varepsilon^t_{n+1}$ and $\xi^r_{n+1} = \xi_n$
- (h) `IF` $\xi_{n+1} \geq 1$, `THEN` set $\xi_{n+1} = 1$, repeat steps (c)-(g) and `EXIT`
- (i) Update transformation surface $\Phi^{t(k+1)}_{n+1}$ using Eq. (10)
- (j) `IF` $\Phi^{t(k+1)}_{n+1} < tolerance$ `THEN EXIT`
- (k) `ELSE` $(k+1) \to k$, `GO TO` (3)(b)

- (l) `IF chck` $= 2$ then correct for reverse transformation
- (m) Calculate $\Delta\xi^k_{n+1}$ from Eq. (31)
- (n) Update $\xi^{(k+1)}_{n+1} = \xi^k_{n+1} + \Delta\xi^k_{n+1}$
- (o) Update $\varepsilon^{t(k+1)}_{n+1}$ using Eq. (40)
- (p) Update $E^{(k+1)}_{n+1}$ using Eq. (4)
- (q) Update $\sigma^{(k+1)}_{n+1}$ using Eq. (5)
- (r) `IF` $\xi_{n+1} = 0$ `THEN` $\xi^r_{n+1} = 0$ and $\varepsilon^{t-r} = 0$
- (s) `IF` $\xi_{n+1} \leq 0$, `THEN` set $\xi_{n+1} = 0$, repeat steps (n)-(r) and `EXIT`
- (t) Update transformation surface $\Phi^{t(k+1)}_{n+1}$ from Eq. (11)
- (u) `IF` $\Phi^{t(k+1)}_{n+1} < tolerance$ `THEN EXIT`
- (v) `ELSE` $(k+1) \to k$, `GO TO` (3)(i)
