

1 Goals and principals

Goals:

- Develop a numerical framework for implementation of general viscoelasticity constitutive models;
- Detail all the required mathematical developments for the model to be defensible against rigorous scrutiny;
- Provide a user friendly library which allows a user to implement their own viscoelastic model with a minimum required effort and understanding of the mathematical developments presented here.

Principals:

- Do as much mathematical development as one can before inserting new information. This creates ‘modular mathematics’ which can be converted into modular code.
- If something can be automated it should be automated.

2 A framework for nonlinear generalized 1D rheological Maxwell networks

2.1 Kinematics and kinetics

Consider the network diagram illustrating the viscoelastic behaviour of a 1D constitutive model in Figure 1. The viscoelastic network

Figure 1

The network diagram implies several axioms for the way in which the components interact:

1. The stress of sequential components is equal;
2. The stress of parallel components is added;
3. The strain of sequential components is added;
4. The strain of parallel components is equal.

Mathematically, these axioms assert that the following equations define the overall constitutive model and that each equation must be satisfied for the constitutive model to be self-consistent:

$$\sigma_i^s = \sigma_i^d = \sigma_i^e, \quad (1)$$

$$\sigma = \sigma^b + \sum_i^n \sigma_i^e, \quad (2)$$

$$\varepsilon_i^e = \varepsilon_i^d + \varepsilon_i^s, \quad (3)$$

$$\varepsilon = \varepsilon_i^e. \quad (4)$$

Note that, for the kinematic state of the network to be completely defined, that is, for the strain of each component to be defined ε , ε_i^d , ε_i^s , ε_i^e , $i = 1, \dots, n$, one needs to define ε and ε_i^d . Then, the other strain values are defined by equations (3) and (4). Hence, we identify ε_i^d as a state variable.

$$\varepsilon = \varepsilon^d + \varepsilon^s. \quad (5)$$

$$\dot{\varepsilon} = \dot{\varepsilon}^d + \dot{\varepsilon}^s. \quad (6)$$

2.2 Thermodynamic considerations

Rate of work done on each Maxwell branch

$$\dot{w}_i^e = \sigma_i^e \dot{\varepsilon} = \underbrace{\sigma_i^s [\dot{\varepsilon} - \dot{\varepsilon}_i^d]}_{\dot{\Psi}_i^e} + \underbrace{\sigma_i^d \dot{\varepsilon}_i^d}_{\dot{\Phi}_i^e} \quad (7)$$

Axioms for the sub-constitutive models

$$1. \sigma_i^s(\varepsilon_i^s), \sigma_i^e(0) = 0$$

$$2. \sigma_i^d(\dot{\varepsilon}_i^d), \sigma_i^d(0) = 0$$

$$\frac{d\Psi_i^e}{d\varepsilon^s} \dot{\varepsilon}^s = \sigma_i^s [\dot{\varepsilon} - \dot{\varepsilon}_i^d] \Rightarrow \left[\frac{d\Psi_i^e}{d\varepsilon^s} - \sigma_i^s \right] \dot{\varepsilon}^s = 0 \Rightarrow \sigma_i^s = \frac{d\Psi_i^e}{d\varepsilon^s} \quad (8)$$

$$D = \sigma_i^e \dot{\varepsilon} - \dot{\Psi}_i^e \geq 0 \quad (9)$$

$$D = \sigma_i^d \dot{\varepsilon}_i^d = \dot{\Phi}_i^e \geq 0 \quad (10)$$

$$\dot{\Psi} = \dot{\Psi}^b + \sum_i^n \dot{\Psi}_i^e \quad (11)$$

2.3 Framework allowing for arbitrary choice of sub-constitutive models

Partition of the time domain

$$0 = t_0 < t_1 < \dots < t_n < t_{n+1} = t \quad (12)$$

Define

$$\Delta t_{n+1} = t_{n+1} - t_n, \quad t_{n+0.5} = \frac{1}{2} [t_{n+1} + t_n] . \quad (13)$$

$$\dot{\varepsilon}_{n+1}^d = \frac{1}{\Delta t_{n+1}} [\varepsilon_{n+1}^d - \varepsilon_n^d] \quad (14)$$

$$\dot{\varepsilon}_{n+1} = \frac{1}{\Delta t_{n+1}} [\varepsilon_{n+1} - \varepsilon_n] \quad (15)$$

$$\sigma^s(\varepsilon_{n+1} - \varepsilon_{n+1}^d) = \sigma^d(\dot{\varepsilon}_{n+1}^d) \quad (16)$$

$$r = \sigma^d(\dot{\varepsilon}_{n+1}^d) - \sigma^s(\varepsilon_{n+1} - \varepsilon_{n+1}^d) \quad (17)$$

$$L[r] = r_i + \frac{dr}{d\varepsilon_{n+1}^d(i)} \Delta \varepsilon_{n+1}^d(i) \quad (18)$$

$$\varepsilon_{n+1(i+1)}^d = \varepsilon_{n+1(i)}^d - \left[\frac{dr}{d\varepsilon_{n+1}^d} \right]_i^{-1} r_i \quad (19)$$

$$\frac{dr}{d\varepsilon_{n+1}^d} = \frac{d\sigma^d}{d\dot{\varepsilon}^d} \frac{d}{d\varepsilon_{n+1}^d} \left[\frac{1}{\Delta t_{n+1}} [\varepsilon_{n+1}^d - \varepsilon_n^d] \right] - \frac{d\sigma^s}{d\varepsilon^s} \frac{d}{d\varepsilon_{n+1}^d} [\varepsilon_{n+1} - \varepsilon_{n+1}^d] \quad (20)$$

$$\frac{dr}{d\varepsilon_{n+1}^d} = \frac{1}{\Delta t_{n+1}} \frac{d\sigma^d}{d\dot{\varepsilon}^d} + \frac{d\sigma^s}{d\varepsilon^s} \quad (21)$$

2.4 Some temporal approximations

2.4.1 Backward difference

2.4.2 An approximation with chosen order of accuracy

$$a(t) = \sum_{i=0}^m \phi_i(t) a_{n+1-i}, \quad \phi_i = \prod_{\substack{j=0 \\ j \neq i}}^m \frac{t - t_{n+1-j}}{t_{n+1-i} - t_{n+1-j}} . \quad (22)$$

$$\dot{a}(t) = \sum_{i=0}^m \dot{\phi}_i(t) a_{n+1-i}, \quad \dot{\phi}_i = \left[\prod_{\substack{j=0 \\ j \neq i}}^m \frac{1}{t_{n+1-i} - t_{n+1-j}} \right] \left[\sum_{\substack{k=0 \\ k \neq i}}^m \prod_{\substack{j=0 \\ j \neq k \\ j \neq i}}^m t - t_{n+1-j} \right] . \quad (23)$$

2.4.3 Stability

$$\dot{\sigma}^d = \dot{\sigma}^s \quad (24)$$

$$\dot{\sigma}^d = \frac{d\sigma^s}{d\varepsilon^s} \dot{\varepsilon}^s \quad (25)$$

2.5 Some constitutive models

2.5.1 Linear models

$$\sigma^\infty = E^\infty \varepsilon \quad (26)$$

$$\sigma^s = E^s [\varepsilon - \varepsilon^d] , \quad \sigma^d = \eta \dot{\varepsilon}^d . \quad (27)$$

$$\sigma^s = \sigma^d \Rightarrow$$

$$E^s [\varepsilon - \varepsilon^d] = \eta \dot{\varepsilon}^d \quad (28)$$

$$\tau = \frac{\eta}{E^s} \quad (29)$$

$$\frac{1}{\tau} \varepsilon = \frac{1}{\tau} \varepsilon^d + \dot{\varepsilon}^d \quad (30)$$

Integrating factor:

$$\exp \left(\int \frac{1}{\tau} dt \right) = \exp \left(\frac{t}{\tau} \right) \quad (31)$$

$$\frac{1}{\tau} \exp \left(\frac{t}{\tau} \right) \varepsilon = \frac{d}{dt} \left[\exp \left(\frac{t}{\tau} \right) \varepsilon^d \right] \quad (32)$$

$$\varepsilon^d = \int_{-\infty}^t \frac{1}{\tau} \exp \left(\frac{s-t}{\tau} \right) \varepsilon ds \quad (33)$$

IBP

$$\varepsilon^d = \varepsilon - \int_{-\infty}^t \exp \left(\frac{s-t}{\tau} \right) \dot{\varepsilon} ds \quad (34)$$

$$\sigma^e = E^s [\varepsilon - \varepsilon^d] = \int_{-\infty}^t \exp \left(\frac{s-t}{\tau} \right) E^s \dot{\varepsilon} ds \quad (35)$$

$$\sigma = \sigma^\infty + \sigma^e = \int_{-\infty}^t \left[E^\infty + \exp \left(\frac{s-t}{\tau} \right) E^s \right] \dot{\varepsilon} ds \quad (36)$$

Integrate by parts ...

Consider three loading conditions

1. Instantaneously applied strain:

$$\varepsilon = \begin{cases} 0 & t < 0 \\ \varepsilon_0 & 0 \leq t \end{cases} \quad (37)$$

2. Instantaneously applied stress:

$$\sigma = \begin{cases} 0 & t < 0 \\ \sigma_0 & 0 \leq t \end{cases} \quad (38)$$

3. Constant strain rate:

$$\varepsilon = \begin{cases} 0 & t < 0 \\ \dot{\varepsilon}_0 t & 0 \leq t \end{cases} \quad (39)$$

4. Cyclical loading at different rates ...

5. Cyclical loading at different rates incrementally increasing max strain -> damage & plasticity

...

Instant strain

Instant stress

Constant strain rate

Fix incorrect sign:

$$\sigma = E^\infty \dot{\varepsilon}_0 t - \tau \left[1 - \exp\left(\frac{-t}{\tau}\right) \right] E^s \dot{\varepsilon}_0 \quad (40)$$

$$\sigma = E^\infty \varepsilon - \tau \left[1 - \exp\left(\frac{-\varepsilon}{\dot{\varepsilon}_0 \tau}\right) \right] E^s \dot{\varepsilon}_0 \quad (41)$$

2.5.2 Ostwald-de Waele model

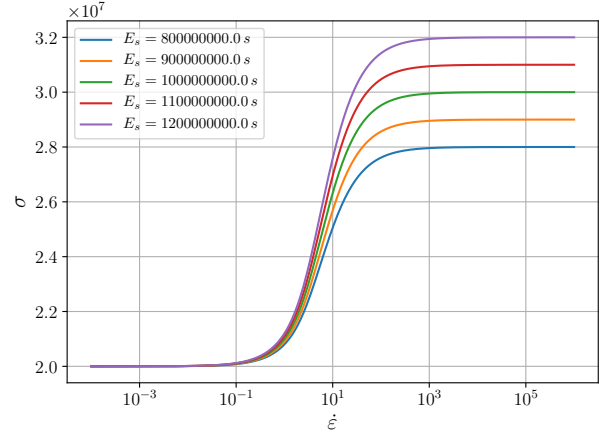
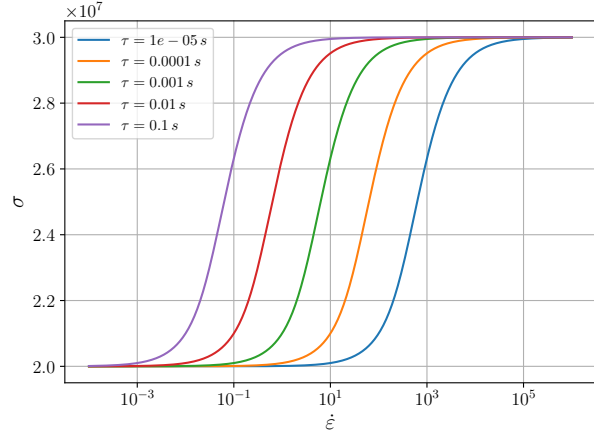
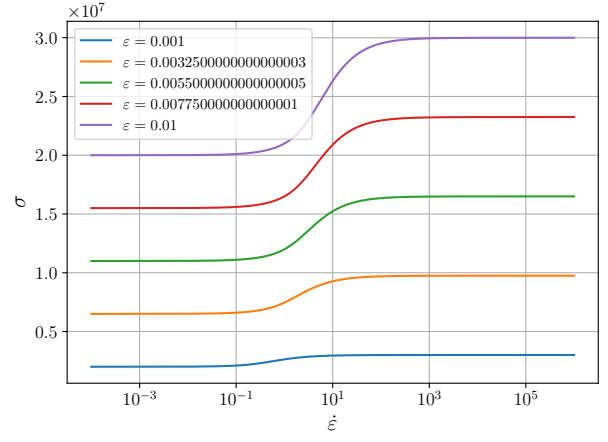
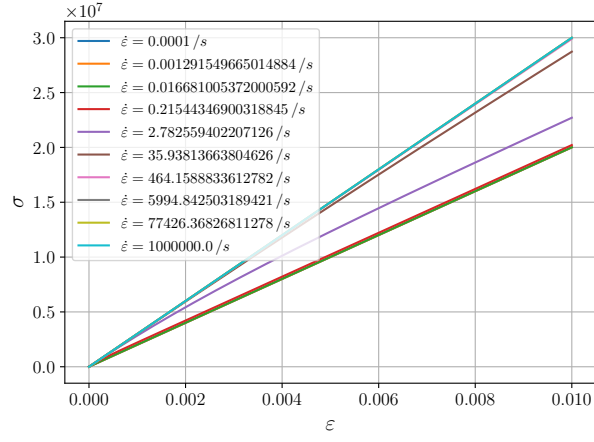
Bone is assumed to be impregnated with blood and other biological fluids which are susceptible to shear thinning or thickening

$$\sigma^d = \eta(\dot{\varepsilon}^d) \dot{\varepsilon}^d \quad (42)$$

$$D = \eta(\dot{\varepsilon}^d) [\dot{\varepsilon}^d]^2 \geq 0, \quad \eta(\dot{\varepsilon}^d) \geq 0. \quad (43)$$

$$\eta(\dot{\varepsilon}^d) = \eta_0 |\dot{\varepsilon}^d|^{n-1} \quad (44)$$

Can change slant. See for example Figure 3.



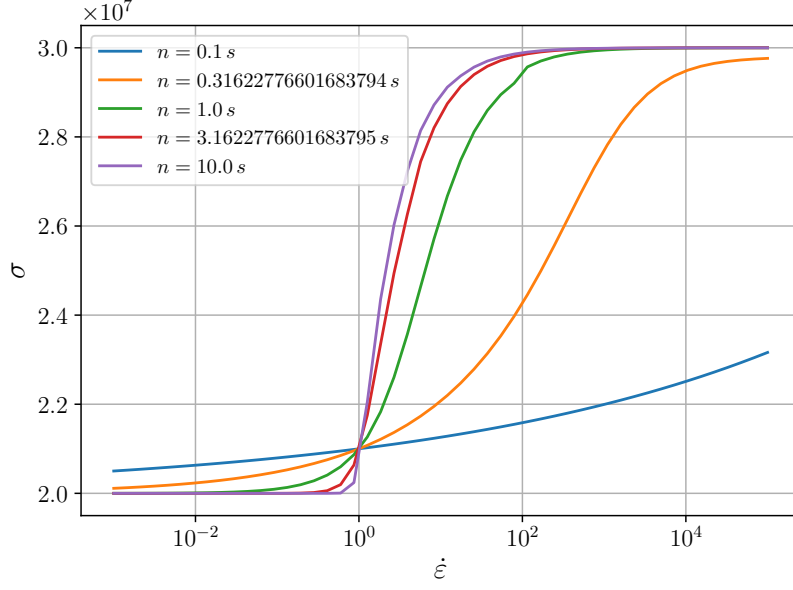


Figure 3

2.5.3 Carreau–Yasuda model

$$\eta = \eta^\infty + [\eta^0 - \eta^\infty] \left[1 + [\lambda |\dot{\epsilon}^d|]^a \right]^{[n-1]/a} \quad (45)$$

3 Going 3D

3.1 Isochoric-volumetric split of the strain

Logic: viscous effects are caused by fluids which are approximated as incompressible (only experience isochoric strains).

$$\boldsymbol{\sigma}^\infty = \lambda \mathbf{I} \text{tr}(\boldsymbol{\epsilon}) + 2\mu \boldsymbol{\epsilon} \quad (46)$$

$$\sigma_{ij}^\infty = \lambda \delta_{ij} \epsilon_{mm} + 2\mu \epsilon_{ij} \quad (47)$$

$$\boldsymbol{\epsilon} = \bar{\boldsymbol{\epsilon}} + \hat{\boldsymbol{\epsilon}}, \quad \hat{\boldsymbol{\epsilon}} = \frac{1}{3} \mathbf{I} \text{tr}(\boldsymbol{\epsilon}) \quad (48)$$

$$\boldsymbol{\sigma}^\infty = \lambda \mathbf{I} \text{tr}(\bar{\boldsymbol{\epsilon}} + \hat{\boldsymbol{\epsilon}}) + 2\mu [\bar{\boldsymbol{\epsilon}} + \hat{\boldsymbol{\epsilon}}] \quad (49)$$

$$\sigma_{ij}^\infty = \lambda \delta_{ij} \hat{\epsilon}_{mm} + 2\mu \hat{\epsilon}_{ij} + 2\mu \bar{\epsilon}_{ij} \quad (50)$$

$$\sigma_{ij}^\infty = \underbrace{[\lambda\delta_{ij}\delta_{kl} + 2\mu\delta_{ik}\delta_{jl}]}_{\hat{\mathbb{C}}_{ijkl}} \hat{\varepsilon}_{kl} + \underbrace{2\mu\delta_{ik}\delta_{jl}}_{\bar{\mathbb{C}}_{ijkl}} \bar{\varepsilon}_{kl} \quad (51)$$

$$\hat{\sigma}_{ij}^\infty = \hat{\mathbb{C}}_{ijkl} \hat{\varepsilon}_{kl}, \quad \bar{\sigma}_{ij}^\infty = \bar{\mathbb{C}}_{ijkl} \bar{\varepsilon}_{kl}$$

3.2 Maxwell network in 3D

Motivated by 1D Maxwell network:

$$\bar{\sigma}_i^s = \bar{\sigma}_i^d = \bar{\sigma}_i^e, \quad (52)$$

$$\bar{\varepsilon}_i = \bar{\varepsilon}_i^d + \bar{\varepsilon}_i^s, \quad (53)$$

$$\bar{\sigma} = \bar{\sigma}^b + \sum_i^n \bar{\sigma}_i^e, \quad (54)$$

$$\hat{\sigma}_i^s = \hat{\sigma}_i^d = \hat{\sigma}_i^e, \quad (55)$$

$$\hat{\varepsilon}_i = \hat{\varepsilon}_i^d + \hat{\varepsilon}_i^s, \quad (56)$$

$$\hat{\sigma} = \hat{\sigma}^b + \sum_i^n \hat{\sigma}_i^e, \quad (57)$$

$$\sigma = \hat{\sigma} + \bar{\sigma}. \quad (58)$$

3.3 Framework

Algorithm 1 Procedure for determining stress and constitutive tensor required by ABAQUS for a compressible material given the derivatives of its strain energy function.

- 1: **procedure** INCREMENT_VISCOELASTIC_MATERIAL(ε^{n+1} , $\bar{\varepsilon}^{d(n)}$)
 - 2: $\hat{\varepsilon} = \frac{1}{3} \mathbf{I} \text{tr}(\varepsilon^{n+1})$
 - 3: $\bar{\varepsilon} = \varepsilon^{n+1} - \hat{\varepsilon}$
 - 4: $\sigma^\infty = 3\lambda\hat{\varepsilon} + 2\mu\varepsilon^{n+1}$
 - 5: $\bar{\sigma}^\infty(:, :, :) = \text{CALC_BIG_A}(\mathbf{F}, \mathbf{a}_0, \mathbf{b}_0)$
 - 6: $J = \det \mathbf{F}$
 - 7: $\sigma = \mathbf{0}$
 - 8: **return** σ, ABA
 - 9: **end procedure**
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3.4 Some models

3.4.1 Linear models

$$\bar{\sigma}_{ij}^\infty = \bar{\mathbb{C}}_{ijkl} \bar{\varepsilon}_{kl} \quad (59)$$

$$\bar{\sigma}_{ij}^d = \bar{\mathbb{C}}_{ijkl}^d \dot{\bar{\epsilon}}_{kl}^d \quad (60)$$

$$\bar{\sigma}_{ij}^s = \bar{\mathbb{C}}_{ijkl}^s [\bar{\epsilon}_{kl} - \bar{\epsilon}_{kl}^d] \quad (61)$$

$$\bar{\mathbb{C}}_{ijkl}^d \dot{\bar{\epsilon}}_{kl}^d = \bar{\mathbb{C}}_{ijkl}^s [\bar{\epsilon}_{kl} - \bar{\epsilon}_{kl}^d] \quad (62)$$

$$\bar{\mathbb{C}}_{ijkl}^d \dot{\bar{\epsilon}}_{kl}^d + \bar{\mathbb{C}}_{ijkl}^s \bar{\epsilon}_{kl}^d = \bar{\mathbb{C}}_{ijkl}^s \bar{\epsilon}_{kl} \quad (63)$$

$$\bar{\mathbb{C}}^d = \tau \bar{\mathbb{C}}^s \quad (64)$$

$$\dot{\bar{\epsilon}}^d + \frac{1}{\tau} \bar{\epsilon}^d = \frac{1}{\tau} \bar{\epsilon} \quad (65)$$

$$\bar{\epsilon}^d = \bar{\epsilon} - \int_{-\infty}^t \exp\left(\frac{s-t}{\tau}\right) \dot{\bar{\epsilon}} \, ds \quad (66)$$

$$\bar{\sigma}^e = \int_{-\infty}^t \exp\left(\frac{s-t}{\tau}\right) \bar{\mathbb{C}}^s \dot{\bar{\epsilon}} \, ds \quad (67)$$

3.4.2 Ostwald-de Waele model

$$\bar{\sigma}^d = \bar{\mathbb{C}}^d \dot{\bar{\epsilon}}^d \quad (68)$$

$$\bar{\mathbb{C}}_{ijop}^d = \eta_0 \left\| \dot{\bar{\epsilon}}^d \right\|^{n-1} \delta_{io} \delta_{jp} \quad (69)$$

$$\frac{\partial \bar{\sigma}_{ij}^d}{\partial \dot{\bar{\epsilon}}_{kl}^d} = \bar{\mathbb{C}}_{ijkl}^d + \left[\frac{\partial}{\partial \dot{\bar{\epsilon}}_{kl}^d} \bar{\mathbb{C}}_{ijop}^d \right] \dot{\bar{\epsilon}}_{op}^d \quad (70)$$

$$\frac{\partial}{\partial \dot{\bar{\epsilon}}_{kl}^d} (\dot{\bar{\epsilon}}_{mn} \dot{\bar{\epsilon}}_{mn})^{[n-1]/2} = [n-1] (\dot{\bar{\epsilon}}_{mn} \dot{\bar{\epsilon}}_{mn})^{[n-3]/2} \dot{\bar{\epsilon}}_{kl} = [n-1] \left\| \dot{\bar{\epsilon}}^d \right\|^{n-3} \dot{\bar{\epsilon}}_{kl} \quad (71)$$

$$\frac{\partial \bar{\sigma}_{ij}^d}{\partial \dot{\bar{\epsilon}}_{kl}^d} = \bar{\mathbb{C}}_{ijkl}^d + [n-1] \left\| \dot{\bar{\epsilon}}^d \right\|^{n-3} \dot{\bar{\epsilon}}_{ij}^d \dot{\bar{\epsilon}}_{kl}^d \quad (72)$$

$$\frac{\partial \bar{\sigma}^d}{\partial \dot{\bar{\epsilon}}^d} = \bar{\mathbb{C}}^d + [n-1] \left\| \dot{\bar{\epsilon}}^d \right\|^{n-3} \dot{\bar{\epsilon}}^d \otimes \dot{\bar{\epsilon}}^d \quad (73)$$

$$\mathbf{r} = \bar{\sigma}^d (\dot{\bar{\epsilon}}_{n+1}^d) - \bar{\sigma}^s (\bar{\epsilon}_{n+1} - \bar{\epsilon}_{n+1}^d) \quad (74)$$

$$\frac{\partial \mathbf{r}}{\partial \bar{\epsilon}_{n+1}^d} = \frac{\partial \bar{\sigma}^d (\dot{\bar{\epsilon}}_{n+1}^d)}{\partial \dot{\bar{\epsilon}}_{n+1}^d} \frac{\partial \dot{\bar{\epsilon}}_{n+1}^d}{\partial \bar{\epsilon}_{n+1}^d} + \frac{\partial \bar{\sigma}^s}{\partial \bar{\epsilon}_{n+1}^s} \quad (75)$$

Algorithm 2 Procedure for determining stress and constitutive tensor required by ABAQUS for a compressible material given the derivatives of its strain energy function.

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1: procedure INCREMENT_VISCOELASTIC_MATERIAL( $\boldsymbol{\varepsilon}$ )
2:    $\mathbf{A}(:, :, :) = \text{CALC\_A}(\mathbf{F}, \mathbf{a}_0, \mathbf{b}_0)$ 
3:    $\mathbb{A}(:, :, :) = \text{CALC\_BIG\_A}(\mathbf{F}, \mathbf{a}_0, \mathbf{b}_0)$ 
4:    $J = \det \mathbf{F}$ 
5:    $\boldsymbol{\sigma} = \mathbf{0}$ 
6:   return  $\boldsymbol{\sigma}_{, \text{ABA}}$ 
7: end procedure

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