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Computational plasticity and viscoplasticity for composite materials and structures

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The paper extends a recently developed theory of mathematical homogenization with eigenstrains to account for viscous effects. A unified mathematical and numerical model of plasticity and viscoplasticity is employed within the framework of the power-law and the Bodner-Partom models.

1.0 Introduction

A typical aerospace composite component can be modeled on (at least) three different scales: (i) macroscale (structural level), (ii) mesoscale (laminate level), and (iii) microscale (the level of microconstituents). Additional scales can be introduced into the model. For example, the scale of material heterogeneity in each microphase, such as dislocations and grain boundaries, could be considered as another scale, not to mention the atomic and electronic scales as the smallest spatial scales.

Computational models can be either deterministic or stochastic. Various deterministic approaches can be classified into the following three categories (i) the classical uncoupled approach [12], [2], [4], [5], [11], [13], (ii) the coupled approach assuming micro/mesostructure periodicity [14], [15], and (iii) the coupled approach free of periodicity assumptions [17], [16], [18].

The uncoupled approach employs representative volume elements (RVE) at one level to produce averaged parameters for the use at the next level. The mathematical homogenization theory [12], [5] provides a theoretical framework for the uncoupled approach. For three or more spatial scales the mathematical homogenization theory has been employed in [13]. The computational complexity of solving nonlinear heterogeneous systems is much greater. While for linear problems the RVE problem has to be solved only once, for nonlinear history dependent systems it has to be solved at every increment and for each integration point. Moreover, history data has to be updated at a number of integration points equal to the product of integration points at all modeling scales considered.

The primary objective of the present manuscript is to extend the recent formulation of the mathematical homogenization theory with eigenstrains developed by the authors in [4] to account for viscous effects. We focus on the uncoupled approach assuming solution periodicity. In Section 2 we derive a closed form expression relating arbitrary transformation fields to mechanical fields in the phases. In Section 3 the 2-point approximation scheme (for two phase materials), where each point represents an average response within a phase is derived. The local response within each phase is recovered by means of post-processing. A unified mathematical and numerical model of plasticity and viscoplasticity is employed within the framework of the power-law [7], [8] and the Bodner-Partom [1], [6], [10] models. Numerical experiments are conducted in Section 4. A discussion on future work conclude the manuscript.

2.0 Mathematical homogenization with eigenstrains

In this section we summarize our recent results on mathematical homogenization with eigenstrains [4]. We regard all inelastic strains, phase transformation as eigenstrains in an otherwise elastic body. Attention is restricted to small deformations. For extensions to large deformation theory we refer to [11].

The microstructure of a composite material is assumed to be locally periodic (Y-periodic) with a periodic arrangement represented by a Unit Cell or a Representative Volume Element, denoted by Θ. Let $\boldsymbol{x}$ be a macroscopic coordinate vector in macro-domain Ω and $\boldsymbol{y} \equiv \boldsymbol{x}/\varsigma$ be a microscopic position vector in Θ. For any Y-periodic function f, we have $f(\boldsymbol{x}, \boldsymbol{y}) = f(\boldsymbol{x}, \boldsymbol{y} + \boldsymbol{k}\hat{\boldsymbol{y}})$ in which vector $\hat{\boldsymbol{y}}$ is the basic period of the microstructure and $\boldsymbol{k}$ is a 3 by 3 diagonal matrix with integer components. Adopting the classical nomenclature, any Y-periodic function f can be represented as

$$f^{\varsigma}(\boldsymbol{x}) \equiv f(\boldsymbol{x}, \boldsymbol{y}(\boldsymbol{x})) \tag{1}$$

where superscript ς denotes a Y-periodic function f. The indirect macroscopic spatial derivatives of f^{ς} can be calculated by the chain rule as

$$f^{\varsigma}_{,x_i}(\boldsymbol{x}) \equiv f_{;x_i}(\boldsymbol{x}, \boldsymbol{y}) = f_{,x_i}(\boldsymbol{x}, \boldsymbol{y}) + \frac{1}{\varsigma} f_{,y_i}(\boldsymbol{x}, \boldsymbol{y}) \tag{2}$$

where a comma followed by a subscript variable x_i or y_i denotes a partial derivative with respect to the subscript variable (i.e. $f_{,x_i} \equiv \partial f/\partial x_i$ or $f_{,y_i} \equiv \partial f/\partial y_i$). A semi-colon followed by a subscript variable x_i denotes a *total* partial derivative with respect to x_i where $\boldsymbol{y}$ depends on $\boldsymbol{x}$, as defined in (2). Summation convention for repeated right hand side subscripts is employed, except for subscripts x and y.

We assume that micro-constituents possess homogeneous properties and satisfy equilibrium, constitutive and kinematical conditions. The corresponding boundary value problem is governed by the following equations:

$$\sigma^{\varsigma}_{ij;x_j} + b_i = 0 \quad \text{in} \quad \Omega \tag{3}$$

$$\sigma^{\varsigma}_{ij} = L_{ijkl}(\varepsilon^{\varsigma}_{kl} - \mu^{\varsigma}_{kl}) \quad \text{in} \quad \Omega \tag{4}$$

$$\varepsilon^{\varsigma}_{ij} = u^{\varsigma}_{(i;x_j)} \equiv \frac{1}{2}(u^{\varsigma}_{i;x_j} + u^{\varsigma}_{j;x_i}) \quad \text{in} \quad \Omega \tag{5}$$

and appropriate set of boundary and interface conditions. In the above equations, σ^{ς}_{ij} and $\varepsilon^{\varsigma}_{ij}$ are components of stress and strain tensors; L_{ijkl} and μ^{ς}_{ij} are components of elastic stiffness and eigenstrain tensors, respectively; b_i is a body force assumed to be independent of $\boldsymbol{y}$; and u^{ς}_i denotes the components of the displacement vector. Subscript pairs with parenthesizes denote symmetric gradients.

In the following, displacements $u^{\varsigma}_i(\boldsymbol{x}) = u_i(\boldsymbol{x}, \boldsymbol{y})$ and eigenstrains $\mu^{\varsigma}_{ij}(\boldsymbol{x}) = \mu_{ij}(\boldsymbol{x}, \boldsymbol{y})$ are approximated in terms of double scale asymptotic expansions on $\Omega \times \Theta$:

$$u_i(\boldsymbol{x}, \boldsymbol{y}) \approx u^0_i(\boldsymbol{x}, \boldsymbol{y}) + \varsigma u^1_i(\boldsymbol{x}, \boldsymbol{y}) + \ldots \tag{6}$$

$$\mu_{ij}(\boldsymbol{x}, \boldsymbol{y}) \approx \mu^0_{ij}(\boldsymbol{x}, \boldsymbol{y}) + \varsigma \mu^1_{ij}(\boldsymbol{x}, \boldsymbol{y}) + \ldots \tag{7}$$

The corresponding expansions of strain and stress tensors can be obtained by manipulating (6), (7), (4) and (5) with consideration of the indirect differentiation rule (2)

$$\varepsilon_{ij}(\boldsymbol{x}, \boldsymbol{y}) \approx \frac{1}{\varsigma}\varepsilon^{-1}_{ij}(\boldsymbol{x}, \boldsymbol{y}) + \varepsilon^0_{ij}(\boldsymbol{x}, \boldsymbol{y}) + \varsigma\varepsilon^1_{ij}(\boldsymbol{x}, \boldsymbol{y}) + \ldots \tag{8}$$

$$\sigma_{ij}(\boldsymbol{x}, \boldsymbol{y}) \approx \frac{1}{\varsigma}\sigma^{-1}_{ij}(\boldsymbol{x}, \boldsymbol{y}) + \sigma^0_{ij}(\boldsymbol{x}, \boldsymbol{y}) + \varsigma\sigma^1_{ij}(\boldsymbol{x}, \boldsymbol{y}) + \ldots \tag{9}$$

where strain components for various orders of ς are given as

$$\varepsilon^{-1}_{ij} = \varepsilon_{yij}(\boldsymbol{u}^0), \qquad \varepsilon^s_{ij} = \varepsilon_{xij}(\boldsymbol{u}^s) + \varepsilon_{yij}(\boldsymbol{u}^{s+1}), \quad s = 0, 1, \ldots \tag{10}$$

and

$$\varepsilon_{xij}(\boldsymbol{u}^s) = u^s_{(i,x_j)}, \qquad \varepsilon_{yij}(\boldsymbol{u}^s) = u^s_{(i,y_j)} \tag{11}$$

Stresses and strains for different orders of ς are related by the following constitutive equations

$$\sigma^{-1}_{ij} = L_{ijkl}\varepsilon^{-1}_{kl}, \qquad \sigma^s_{ij} = L_{ijkl}(\varepsilon^s_{kl} - \mu^s_{kl}), \quad s = 0, 1, \ldots \tag{12}$$

Inserting the stress expansion (9) into equilibrium equation (3) and making the use of (2) yields a set of equilibrium equations for various orders [4]. From the lowest order $O(\varsigma^{-2})$ equilibrium equation we get $u^0_{(i,y_j)} = 0$ which implies

$$u_i^0 = u_i^0(x) \quad \text{and} \quad \sigma_{ij}^{-1}(x, y) = \varepsilon_{ij}^{-1}(x, y) = 0 \tag{13}$$

In order to solve the $O(\varsigma^{-1})$ equilibrium equation for up to a constant we introduce the following separation of variables

$$u_i^1(x, y) = H_{ikl}(y)\{\varepsilon_{xkl}(u^0) + d_{kl}^{\mu}(x)\} \tag{14}$$

where H_{ikl} is a Y-periodic function, and d_{kl}^{μ} is a macroscopic portion of the solution resulting from eigenstrains, i.e. if $\mu_{kl}^0(x, y) = 0$ then $d_{kl}^{\mu}(x) = 0$. It should be noted that both H_{ikl} and d_{kl}^{μ} are symmetric with respect to indices k and l. Based on (14) the $O(\varsigma^{-1})$ equilibrium equation takes the following form:

$$\{L_{ijkl}((I_{klmn} + H_{(k,y_l)mn})\varepsilon_{xmn}(u^0) + H_{(k,y_l)mn}d_{mn}^{\mu}(x) - \mu_{kl}^0)\}_{,y_j} = 0 \quad \text{on} \quad \Theta \tag{15}$$

where

$$I_{klmn} = \frac{1}{2}(\delta_{mk}\delta_{nl} + \delta_{nk}\delta_{ml}) \tag{16}$$

and δ_{mk} is the Kronecker delta. Since equation (15) is valid for arbitrary combination of macroscopic strain field $\varepsilon_{xmn}(u^0)$ and eigenstrain field μ_{kl}^0, we first consider $\mu_{kl}^0 \equiv 0$, $\varepsilon_{xmn}(u^0) \neq 0$ and then $\varepsilon_{xmn}(u^0) \equiv 0$, $\mu_{kl}^0 \neq 0$ which yields the following two governing equations on Θ:

$$\{L_{ijkl}(I_{klmn} + H_{(k,y_l)mn})\}_{,y_j} = 0 \tag{17}$$

$$\{L_{ijkl}(H_{(k,y_l)mn}d_{mn}^{\mu} - \mu_{kl}^0)\}_{,y_j} = 0 \tag{18}$$

Equation (17) together with Y-periodic boundary conditions comprise a standard linear boundary value problem on Θ. For complex microstructures a finite element method is often employed for discretization of $H_{ikl}(y)$, which yields a set of linear algebraic system with six right hand side vectors [3].

After solving (17) for H_{imn}, the elastic homogenized stiffness $\bar{L}_{ijkl}$ follows from the $O(\varsigma^0)$ equilibrium equation [3]:

$$\bar{L}_{ijkl} \equiv \frac{1}{|\Theta|}\int_{\Theta} L_{ijmn}A_{mnkl}\, d\Theta = \frac{1}{|\Theta|}\int_{\Theta} A_{mnij}L_{mnst}A_{stkl}\, d\Theta \tag{19}$$

where

$$A_{klmn} = I_{klmn} + H_{(k,y_l)mn} \tag{20}$$

A_{klmn} is often referred to as an elastic strain concentration function and $|\Theta|$ is the volume of a unit cell.

A close form expression for d^{μ}_{kl} follows from (18) and (19):

$$d^{\mu}_{ij} = \frac{1}{|\Theta|}(\tilde{L}_{ijkl} - \bar{L}_{ijkl})^{-1}\int_{\Theta} H_{(m,y_n)kl}L_{mnst}\mu^{0}_{st}\, d\Theta \tag{21}$$

where

$$\tilde{L}_{ijkl} = \frac{1}{|\Theta|}\int_{\Theta} L_{ijkl}\, d\Theta \tag{22}$$

The superscript -1 denotes a reciprocal tensor. In the case of piecewise constant eigenstrains [2], the average strain (8) over a subdomain ρ is given as:

$$\varepsilon^{\rho}_{ij} \equiv \frac{1}{|\Theta^{\rho}|}\int_{\Theta^{\rho}} \varepsilon_{ij}\, d\Theta = A^{\rho}_{ijkl}\bar{\varepsilon}_{kl} + \sum_{\eta=1}^{n} F^{\rho\eta}_{ijkl}\mu^{\eta}_{kl} + O(\varsigma) \tag{23}$$

where $F^{\rho\eta}_{ijkl}$ are the eigenstrains influence factors:

$$F^{\rho\eta}_{ijkl} = c^{\eta}(A^{\rho}_{ijmn} - I_{ijmn})(\tilde{L}_{mnpq} - \bar{L}_{mnpq})^{-1}(A^{\eta}_{rspq} - I_{rspq})L^{\eta}_{rskl} \tag{24}$$

and

$$A^{\rho}_{ijkl} = \frac{1}{|\Theta^{\rho}|}\int_{\Theta^{\rho}} (I_{ijkl} + H_{(i,y_j)kl})\, d\Theta \tag{25}$$

The superscripts ρ (or η) denote the ρ-th subdomain, Θ^{ρ}, and n is the total number of subdomains in the unit cell domain. The subdomain could be made of a single finite element or a group of elements; c^{η} is the η-th subdomain volume fraction given by $c^{\eta} \equiv |\Theta^{\eta}|/|\Theta|$ and satisfying $\sum_{\eta=1}^{n} c^{\eta} = 1$.

We refer to the piecewise constant model defined by (23) as the n-point scheme model. As a special case we consider a composite medium consisting of two phases, matrix and reinforcement, with respective volume fractions c^m and c^f such that $c^m + c^f = 1$. Superscripts m and f represent matrix and reinforcement phases, respectively. Θ^m and Θ^f denote the matrix and reinforcement domains such that $\Theta = \Theta^m \cup \Theta^f$. We assume that eigenstrains and elastic strain concentration factors are constant within each phase. This yields the simplest variant of (23) where $n = 2$. The corresponding approximation scheme is termed as the 2-point model. The overall elastic properties are given as:

$$\bar{L}_{ijkl} = c^m L^m_{ijmn} A^m_{mnkl} + c^f L^f_{ijmn} A^f_{mnkl} \tag{26}$$

The influence factors $F^{\rho\eta}_{ijkl}$ reduce to

$$\left.\begin{aligned} F^{\rho m}_{ijkl} &= (I_{ijmn} - A^{\rho}_{ijmn})(L^m_{mnst} - L^f_{mnst})^{-1} L^m_{stkl} \\ F^{\rho f}_{ijkl} &= (I_{ijmn} - A^{\rho}_{ijmn})(L^f_{mnst} - L^m_{mnst})^{-1} L^f_{stkl} \end{aligned}\right\} \qquad \rho = m, f \tag{27}$$

and the overall stress is given as:

$$\bar{\sigma}_{ij} = c^m \sigma^m_{ij} + c^f \sigma^f_{ij} \tag{28}$$

3.0 The 2-point scheme

We consider a two-phase composite where the matrix phase behaves as a rate-dependent or rate independent elastoplastic material, whereas the reinforcement is elastic, i.e. $\mu^f_{ij} = 0$. A unified mathematical and numerical model of plasticity and viscoplasticity for the matrix phase is subsequently described.

3.1 The 2-phase medium

Combining equations (4) and (23) phase stresses can be expressed as:

$$\sigma^{\rho}_{ij} = R^{\rho}_{ijkl} \bar{\varepsilon}_{kl} - Q^{\rho m}_{ijkl} \mu^m_{kl} \tag{29}$$

where μ^m_{kl} is the matrix plastic strain and

$$\left.\begin{aligned} R^{\rho}_{ijkl} &= L^{\rho}_{ijpq} A^{\rho}_{pqkl} \\ Q^{\rho\eta}_{ijkl} &= L^{\rho}_{ijpq}(\delta_{\rho\eta} I_{pqkl} - F^{\rho\eta}_{pqkl}) \end{aligned}\right\} \qquad \rho, \eta = m, f \tag{30}$$

A unified rate-dependent / rate-independent flow rule is given as

$$\dot{\mu}^m_{ij} = \aleph^m_{ij} \dot{\lambda}^m \tag{31}$$

where

$$\aleph_{ij}^m = \frac{\xi_{ij}^m}{\sqrt{\xi_{mn}^m \xi_{mn}^m}}, \qquad \xi_{ij}^m = P_{ijkl}(\sigma_{kl}^m - \alpha_{kl}^m) \tag{32}$$

and $\dot{\mu}_{ij}^m$ represents the plastic strain rate in the matrix phase; $P_{ijkl} = I_{ijkl} - \delta_{ij}\delta_{kl}/3$ is a projection operator which transforms an arbitrary symmetric second order tensor to the deviatoric space; and α_{ij}^m is a back stress. A unified rate-dependent / rate independent consistency condition can be expressed as:

$$\Phi^m \equiv \xi^m - g(\lambda^m, \dot{\lambda}^m) = 0 \tag{33}$$

where ξ^m is an effective stress defined as

$$\xi^m \equiv \sqrt{\frac{3}{2}\xi_{mn}^m \xi_{mn}^m} \tag{34}$$

Attention is restricted to two widely used classes of flow functions:

- The power-law model [7], [8]:

$$\dot{\lambda}^m = a\left(\frac{\xi^m}{Y}\right)^{\frac{1}{b}} \quad \Rightarrow \quad g = Y\left(\frac{\dot{\lambda}^m}{a}\right)^b \tag{35}$$

- The Bodner-Partom model [1], [6], [10]:

$$\dot{\lambda}^m = a\exp\left\{-\frac{1}{2}\left(\frac{Y}{\xi^m}\right)^b\right\} \quad \Rightarrow \quad g = Y\left\{-2\log\left(\frac{\dot{\lambda}^m}{a}\right)\right\}^b \tag{36}$$

where a and b are material constants; Y is a drag or yield stress which is a function of λ^m. The back stress α_{ij}^m is assumed to be governed by the following evolution equation

$$\dot{\alpha}_{ij}^m = \frac{2}{3}H(\lambda^m, \dot{\lambda}^m)\,\dot{\mu}_{ij}^m \tag{37}$$

in which H is a kinematic hardening modulus, which in general depends on the effective plastic strain λ^m and its rate of change $\dot{\lambda}^m$. For simplicity, in the present manuscript H is assumed to be constant. The rate-independent plasticity model can be obtained by taking $b = 0$.

3.2 Implicit Integration of Constitutive Equations

The constitutive equations are integrated over a finite time step Δt using a backward Euler scheme, which yields:

$$^{t+\Delta t}\mu_{ij}^m = {}^t\mu_{ij}^m + \Delta\lambda^m \, {}^{t+\Delta t}\aleph_{ij}^m \tag{38}$$

$$ {}^{t+\Delta t}\alpha_{ij}^{m} = {}^{t}\alpha_{ij}^{m} + \frac{2}{3}\Delta\lambda^{m} H \, {}^{t+\Delta t}\aleph_{ij}^{m} \tag{39} $$

where $\Delta\lambda^{m} \equiv {}^{t+\Delta t}\lambda^{m} - {}^{t}\lambda^{m}$.

In the following we omit the left superscript for the current step $t + \Delta t$ for simplicity. Substituting (38) into (29) yields:

$$ \sigma_{ij}^{m} = {}_{tr}\sigma_{ij}^{m} - \Delta\lambda^{m} Q_{ijkl}^{mm} \aleph_{kl}^{m} \tag{40} $$

where ${}_{tr}\sigma_{ij}^{m}$ is a trial stress in the matrix phase defined as

$$ {}_{tr}\sigma_{ij}^{m} \equiv {}^{t}\sigma_{ij}^{m} + R_{ijkl}^{m} \Delta\bar{\varepsilon}_{kl} \tag{41} $$

Subtracting (39) from (40), we arrive at the following result:

$$ \sigma_{ij}^{m} - \alpha_{ij}^{m} = (I_{ijkl} + \Delta\lambda^{m} \wp_{ijkl})^{-1} ({}_{tr}\sigma_{kl}^{m} - {}^{t}\alpha_{kl}^{m}) \tag{42} $$

where

$$ \wp_{ijkl} = Q_{ijst}^{mm} P_{stkl} + \frac{2}{3} H P_{ijkl} \tag{43} $$

Integrating $\dot{\lambda}^{m}$ using backward Euler scheme, $\lambda^{m} = {}^{t}\lambda^{m} + \dot{\lambda}^{m}\Delta t$, or $\dot{\lambda}^{m} = \Delta\lambda^{m}/\Delta t$, and then combining equations (35) and (36) with the generalized consistency condition in the matrix phase (33) yields:

$$ \text{Power law:} \quad \Phi^{m} \equiv \xi^{m} - Y \left\{ \frac{\Delta\lambda^{m}}{a\Delta t} \right\}^{b} = 0 $$

$$ \text{Bodner-Partom:} \quad \Phi^{m} \equiv \xi^{m} - Y \left\{ -2 \log\left(\frac{\Delta\lambda^{m}}{a\Delta t} \right) \right\}^{b} = 0 \tag{44} $$

The value of $\Delta\lambda^{m}$ is obtained by satisfying the generalized consistency condition (44). For calculation of $\Delta\lambda^{m}$, equation (42) is substituted into (44), which produces a nonlinear equation for $\Delta\lambda^{m}$. The Newton method is applied to solve for $\Delta\lambda^{m}$:

$$ \Delta\lambda_{k+1}^{m} = \Delta\lambda_{k}^{m} - \left\{ \frac{\partial\Phi^{m}}{\partial\Delta\lambda^{m}} \right\}^{-1} \Phi^{m} \Bigg|_{\Delta\lambda_{k}^{m}} \tag{45} $$

where k is an iteration count. It can be shown that the derivative $\partial\Phi^m/\partial\Delta\lambda^m$ required in (45) has the following form:

$$\frac{\partial\Phi^m}{\partial\Delta\lambda^m} = \frac{d\xi^m}{d\Delta\lambda^m} - \frac{dg}{d\Delta\lambda^m}$$

$$\text{Power law:} \quad \frac{dg}{d\Delta\lambda^m} = \left\{\frac{\Delta\lambda^m}{a\Delta t}\right\}^b \left\{\frac{dY}{d\Delta\lambda^m} + \frac{bY}{\Delta\lambda^m}\right\}$$

$$\text{Bodner-Partom:} \quad \frac{dg}{d\Delta\lambda^m} = \left\{-2\log\left(\frac{\Delta\lambda^m}{a\Delta t}\right)\right\}^b \left\{\frac{dY}{d\Delta\lambda^m} + \frac{b}{\Delta\lambda^m \log\left(\frac{\Delta\lambda^m}{a\Delta t}\right)}\right\} \tag{46}$$

where

$$\frac{d\xi^m}{d\Delta\lambda^m} = -\frac{3}{2\xi^m}\xi^m_{ij}(I_{ijkl} + \Delta\lambda^m \wp_{ijkl})^{-1}\wp_{klmn}\xi^m_{mn} \tag{47}$$

and $dY/d\Delta\lambda^m$ is a rate-independent isotropic hardening modulus. The converged value of $\Delta\lambda^m$ is used to compute the phase stresses from equations (42), (38), (29) and the back stress from (39). The overall stress is computed from (28).

3.3 Consistent Linearization

While integration of the constitutive equations affects the accuracy of the solution, the formation of a tangent stiffness matrix consistent with the integration procedure is essential to maintain the quadratic rate of convergence if one is to adopt the Newton method for the solution of nonlinear system of equations on the macro level [9].

The starting point is the incremental form of the phase constitutive equations (29):

$$\Delta\sigma^p_{ij} = R^p_{ijkl}\Delta\bar{\varepsilon}_{kl} - Q^{pm}_{ijkl}\Delta\mu^m_{kl} \tag{48}$$

Taking the material time derivative of (48) and keeping in mind that all quantities are known at the previous step yields

$$\dot{\sigma}^p_{ij} = R^p_{ijkl}\dot{\bar{\varepsilon}}_{kl} - Q^{pm}_{ijkl}\{\Delta\lambda^m \dot{\aleph}^m_{kl} + \dot{\lambda}^m \aleph^m_{kl}\} \tag{49}$$

where

$$\dot{\aleph}^m_{ij} = \Xi_{ijkl}(\dot{\sigma}^m_{kl} - \dot{\alpha}^m_{kl}), \qquad \Xi_{ijkl} = \frac{1}{\xi^m}\sqrt{\frac{3}{2}}(P_{ijmn} - \aleph^m_{ij}\aleph^m_{mn}) \tag{50}$$

To calculate $\dot{\lambda}^m$ we first linearize equation (42)

$$\dot{\sigma}_{ij}^m - \dot{\alpha}_{ij}^m = \Lambda_{ij}\dot{\lambda}^m, \qquad \Lambda_{ij} = -(I_{ijkl} + \Delta\lambda^m \wp_{ijkl})^{-1} \wp_{klmn}\xi_{mn}^m \tag{51}$$

and then substitute (51) into the linearized form of (39), which yields

$$\dot{\alpha}_{ij}^m = \frac{2}{3}H(\Delta\lambda^m \Xi_{ijkl}\Lambda_{kl} + \aleph_{ij}^m)\dot{\lambda}^m \tag{52}$$

Subsequently, we linearize the generalized consistency condition (44)

$$\dot{\Phi}^m = \sqrt{\frac{3}{2}}\aleph_{kl}^m(\dot{\sigma}_{kl}^m - \dot{\alpha}_{kl}^m) - \dot{g} = 0$$

$$\text{Power law:} \quad \dot{g} = \dot{\lambda}^m \left\{\frac{\Delta\lambda^m}{a\Delta t}\right\}^b \left\{\frac{dY}{d\lambda^m} + \frac{bY}{\Delta\lambda^m}\right\}$$

$$\text{Bodner-Partom:} \quad \dot{g} = \dot{\lambda}^m \left\{-2\log\left(\frac{\Delta\lambda^m}{a\Delta t}\right)\right\}^b \left\{\frac{dY}{d\Delta\lambda^m} + \frac{b}{\Delta\lambda^m \log\left(\frac{\Delta\lambda^m}{a\Delta t}\right)}\right\} \tag{53}$$

and then combine (52) and (53) to get the expression for $\dot{\lambda}^m$:

$$\dot{\lambda}^m = \gamma \aleph_{kl}^m \dot{\sigma}_{kl}^m$$

$$\text{Power law:} \quad \gamma = \left(\frac{2}{3}H + \sqrt{\frac{2}{3}}\left\{\frac{\Delta\lambda^m}{a\Delta t}\right\}^b \left\{\frac{dY}{d\lambda^m} + \frac{bY}{\Delta\lambda^m}\right\}\right)^{-1}$$

$$\text{Bodner-Partom:} \quad \gamma = \left(\frac{2}{3}H + \sqrt{\frac{2}{3}}\left\{-2\log\left(\frac{\Delta\lambda^m}{a\Delta t}\right)\right\}^b \left\{\frac{dY}{d\Delta\lambda^m} + \frac{b}{\Delta\lambda^m \log\left(\frac{\Delta\lambda^m}{a\Delta t}\right)}\right\}\right)^{-1} \tag{54}$$

The rate of phase stress can now be expressed as

$$\dot{\sigma}_{ij}^\rho = R_{ijkl}^\rho \dot{\bar{\varepsilon}}_{kl} - \gamma Q_{ijkl}^{\rho m}(\Delta\lambda^m \Xi_{klmn}\Lambda_{mn} + \aleph_{kl}^m)\aleph_{st}^m \dot{\sigma}_{st}^m \tag{55}$$

Evaluating (55) for the matrix phase, $\rho = m$, gives

$$\dot{\sigma}_{ij}^m = D_{ijkl}^m \dot{\bar{\varepsilon}}_{kl} \tag{56}$$

where

$$D^m_{ijkl} = \{I_{ijst} + \gamma Q^{mm}_{ijpq}(\Delta\lambda^m \Xi_{pqmn}\Lambda_{mn} + \aleph^m_{pq})\aleph^m_{st}\}^{-1} R^m_{stkl} \tag{57}$$

Starting from (49) and proceeding in an analogous manner for the rate of the reinforcement stress yields

$$\dot{\sigma}^f_{ij} = D^f_{ijkl}\dot{\bar{\varepsilon}}_{kl} \tag{58}$$

where

$$D^f_{ijkl} = R^f_{ijkl} - \gamma Q^{fm}_{ijpq}(\Delta\lambda^m \Xi_{pqmn}\Lambda_{mn} + \aleph^m_{pq})\aleph^m_{st} D^m_{stkl} \tag{59}$$

The overall consistent instantaneous stiffness $\bar{D}_{ijkl}$ is obtained from the rate form of (28), (56) and (58)

$$\dot{\bar{\sigma}}_{ij} = \bar{D}_{ijkl}\dot{\bar{\varepsilon}}_{kl} \tag{60}$$

where

$$\bar{D}_{ijkl} = c^m D^m_{ijkl} + c^f D^f_{ijkl} \tag{61}$$

3.4 Consistent tangent stiffness matrix

We start from the system of nonlinear equations arising from the finite element discretization

$$r_A = f^{int}_A(q_A) - f^{ext}_A = 0 \qquad f^{int}_A = \int_\Omega N_{iA,x_j}\bar{\sigma}_{ij}d\Omega \tag{62}$$

where N_{kA} is set of C^0 continuous shape functions, such that $v_k = N_{kA}\dot{q}_A$; the upper case subscripts denote the degree-of-freedom and the summation convention over repeated indexes is employed for the degrees-of-freedom and for the spatial dimensions; q_A and $\dot{q}_A$ are components of nodal displacement and velocity vectors; f^{int}_A and f^{ext}_A are components of the internal and external force vectors, respectively.

The consistent tangent stiffness matrix, K_{AB}, is obtained via consistent linearization of the discrete equilibrium equations (62). It is convenient to formulate such a linearization procedure as:

$$K_{AB} \equiv \frac{\partial}{\partial \dot{q}_B}\left(\frac{d}{dt} r_A\right) \qquad (63)$$

For simplicity, assuming that the external force vector is not a function of the solution, the consistent linearization procedure for small deformation theory yields:

$$K_{AB} = \int_{\Omega} N_{iA, x_j} \overline{D}_{ijkl} N_{kB, x_l} \, d\Omega \qquad (64)$$

where $\overline{D}_{ijkl}$ is defined in (61);

Remark: In the 2-point scheme described in Section 3 the eigenstrains have been approximated by a constant within each phase. A better resolution of local fields can be obtained by approximating eigenstrains as piecewise constant within each phase. In [4], the eigenstrains have been assumed to be constant within each element in the unit cell, giving rise to the so called n-point scheme. Typically, the computational cost resulting from the n-point scheme is orders of magnitude higher then that of the 2-point scheme since the number of nonlinear equations to be solved at each macro-Gauss point is equal to the number of Gauss points in a unit cell experiencing inelastic deformation. Therefore, it is advantageous to merge the two approaches. In such a combined scheme the overall structural response is computed using the 2-point scheme, while local fields of interest in the unit cell corresponding to the critical regions in the macro-domain are recovered by means of the n-point scheme [4]. An alternative procedure has been presented in [11].

4.0 Numerical experiments

We consider two numerical examples to test the accuracy and efficiency of the computational schemes. For both examples, continuous fibre microstructure shown in Figure 1 is considered. The unit cell is discretized with 98 tetrahedral elements in the reinforcement domain and 253 in the matrix domain, totaling 330 degrees of freedom.

4.1 The nozzle flap problem

The finite element mesh for one-half of the nozzle flap (due to symmetry) is shown in Figure 2. The mesh contains 788 linear tetrahedral elements (993 degrees of freedom). The flap is subjected to an aerodynamic force (simulated by a uniform pressure) on the back of the flap and a symmetric boundary condition is applied on the symmetric face. We assume that the pin-eyes are rigid and a rotation is not allowed so that all the degrees of freedom on the pin-eye surfaces are fixed. There is about 15 percent of plastic zone in the model due to the loading. The nozzle flap problem is solved using the 2-point averaging scheme with micro-history recovery and the n-point procedures for the reference solution. The objective of this numerical study is to investigate the 2-point averaging scheme with micro-history recovery in terms of accuracy (in both macro- and micro-scales), computational efficiency and memory consumption.

The phase properties are given as follows:

Titanium Matrix: Young's modulus = 68.9 GPa, Poisson's ratio = 0.33,
initial yield stress is 24 MPa, isotropic hardening modulus is 14 GPa
kinematic hardening modulus is 0 GPa

SiC Fiber: Young's modulus = 379.2 GPa, Poisson's ratio = 0.21,
fiber volume fraction is 0.27

For this problem, the power law is adopted with $a = 1$ and $b = 0.1$. The CPU time is 30 seconds for the macroscopic analysis using the 2-point scheme, plus approximately 170 seconds for each Gaussian point where a micro-history recovery procedure is applied. On the other hand, the CPU time for the n-point scheme is over 7 hours. Moreover, memory requirement ratio for these two approaches is roughly 1:250.

Effective micro-stresses obtained by both approaches are compared using the relative error measure defined as

$$Error = 100\frac{\xi^{n-point} - \xi^{2-point}}{\xi^{n-point}} \tag{65}$$

where $\xi^{n-point}$ and $\xi^{2-point}$ are the effective micro-stresses obtained via the n-point and the 2-point schemes, respectively. The maximum effective stress appears at the pin-eye of the middle flap (Gaussian point A). Micro-history is recovered for the unit cell corresponding to the macro Gauss point A. The relative error at this point is approximately 5%, as shown in Figure 3.

4.2 Thick-walled cylinder problem

For our second test problem we consider a composite thick-walled cylinder with an inner radius r_{inner}, and outer radius r_{outer}. The ratio of r_{outer} to r_{inner} is taken to be 2. The finite element discretization is shown in Figure 4. Boundary conditions are assigned in such a way that plain strain and axisymmetric conditions are preserved. A constant displacement rate of 0.002 is imposed on the inner wall of the cylinder. A power law is employed with both the kinematic and isotropic hardening taken to be zero, i.e., $Y(\lambda^m) = Y_0$. Other material constants employed are:

Matrix: Youngs modulus $= 500Y_0$, Poisson ratio $= 0.499$, $a = 0.002$, $b = 0.2$

Fiber: Youngs modulus $= 5000Y_0$, Poisson ratio $= 0.21$

An exact solution for the steady state problem for the homogeneous material ($c^f = 0$) is available in [8]. The inner wall pressures vs. time as obtained with various fiber volume fractions are depicted in Figure 5. The relative error for the steady state problem with $c^f = 0$ is less than 1%.

5.0 Future work

An uncoupled two-scale approach assuming solution periodicity in inelastic heterogeneous media has been presented. The two issues that have not been addressed in the present manuscript are:

i. Stochastic nature of data

So far only the deterministic aspect has been considered. The deterministic approach utilizes mean values associated with microstructural characteristics. The uncertainties in input data pose a tremendous challenge not only because we have to deal with numerical methods for stochastic differential equations [19], but more importantly, because the probability fields, especially the correlations, are usually unknown.

ii. Multiple time scales

The difficulty of estimating the average behavior at the larger length scales from the essential physics at smaller scales is compounded in time dependent problems. Multiple length and time scales can be accounted for by incorporating them into appropriate asymptotic expansions.

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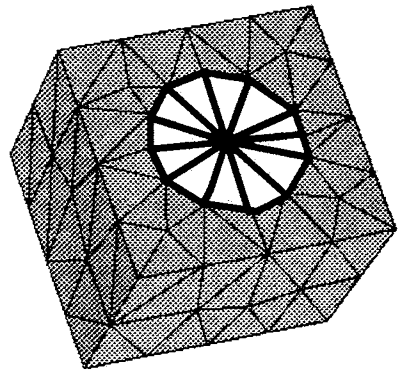

Figure 1: Unit cell discretization

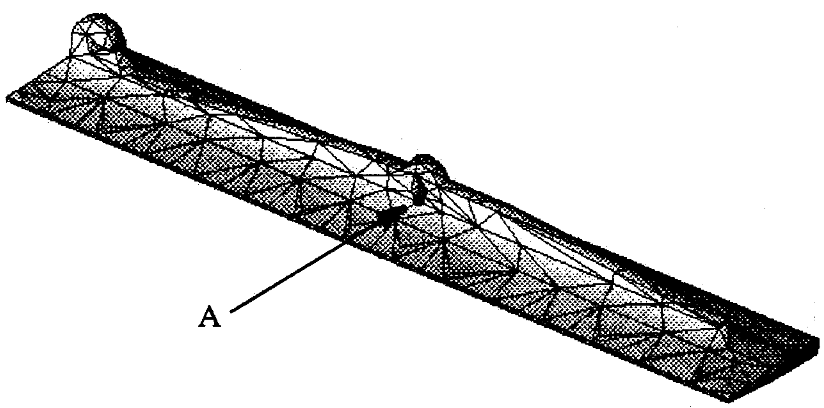

Figure 2: Finite element mesh for the nozzle flap problem

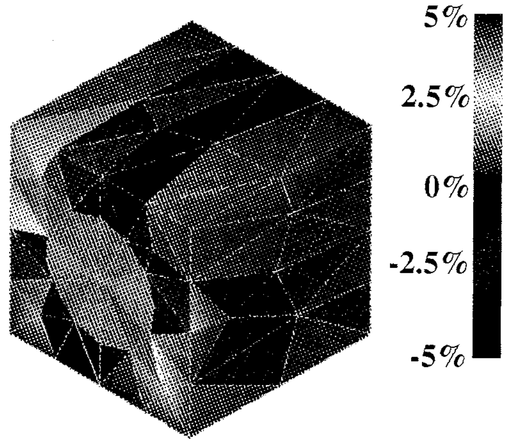

Figure 3: Relative error (%) in effective stress at macro Gauss point A

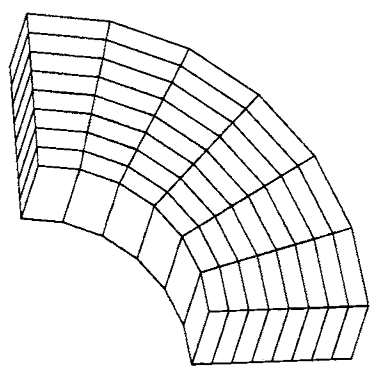

Figure 4: Finite element mesh for the thick-walled cylinder problem

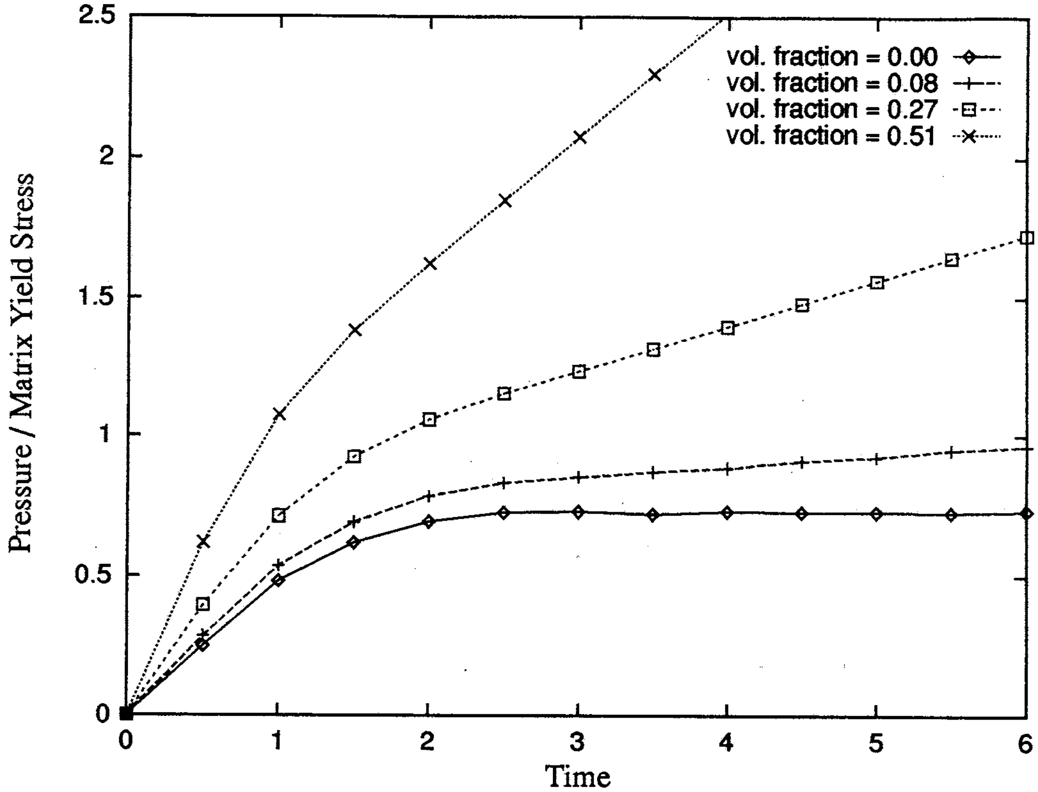

Figure 5: Inner wall pressure vs. time