*A Cell Model for Homogenization
of Fiber-Reinforced Composites:
General Theory and Nonlinear
Elasticity Effects*

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*A Cell Model for Homogenization
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General Theory and Nonlinear
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*John B. Aidun
Frank L. Addessio*

Los Alamos
NATIONAL LABORATORY

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A CELL MODEL FOR HOMOGENIZATION OF FIBER-REINFORCED COMPOSITES:
GENERAL THEORY AND NONLINEAR ELASTICITY EFFECTS

by

John B. Aidun and Frank L. Addessio

ABSTRACT

The theoretical basis of the homogenization technique developed by Aboudi is presented and assessed. Given the constitutive relations of the constituents, this technique provides an equivalent, homogeneous, constitutive model of unidirectional, continuous-fiber-reinforced composites. The expressions that comprise the first-order version of the technique are given special attention as this treatment has considerable practical value. Nonlinear elasticity effects are added to it. This extension increases the accuracy of numerical simulations of high strain-rate loadings. It is particularly important for any dynamic loading in which shock waves might be produced, including crash safety, armor, and munitions applications. Examples illustrate that elastic nonlinearity can make substantial contributions at strains of only a few per cent. These contributions are greatest during post-yield inelastic deformation. The micromechanics-based homogenization technique is shown to facilitate use of an efficient approximate treatment of elastic nonlinearity in composites with isotropic matrix materials.

I. INTRODUCTION

Considerable interest exists in using engineered composite materials to develop lighter structures that are strong under adverse conditions such as high temperature, thermal cycling, vibration and mechanical cycling, and chemical corrosion. Due to the potential capability to tailor the mechanical properties of fiber-reinforced matrices of metal, polymer, or ceramic, these engineered composites are attractive candidates for use in many commercial

automotive, aerospace, and electronics applications, as well as in defense applications including weapons, armor, and munitions. Research leading to application of a composite requires numerical simulations of its response to assist in interpreting mechanical experiments used to characterize it, as well as for designing the structure it composes. It is often desirable to represent a composite with an equivalent, homogeneous-continuum material model in these numerical simulations. Large-scale response simulations, for example, cannot use fine computational meshes to resolve the material microstructure. Consequently, all significant effects of the microstructure on the overall (macroscopic) mechanical response must be accounted for in an equivalent, homogeneous constitutive model of the composite. Though homogeneous, such models often must be elastically and inelastically anisotropic to represent the heterogeneous material adequately. This report describes one method for generating equivalent, homogeneous material models, known as the Method of Cells (MoC),¹ and the addition to it of nonlinear elasticity to better suit it for simulations of high strain rate and high stress response.

The MoC was chosen because of its demonstrated versatility.¹ It is independent of particular stress configurations or structural designs, easy to use, and compatible with arbitrary constitutive relations for intact constituent material. It has been applied to calculate thermo-inelastic response of a variety of engineered composites with good success. The method is applicable to any ordered composite that can be idealized with a microstructural representative volume element (RVE) that generates the entire composite through periodic repetition. A typical RVE comprises a number of subcells. In a continuous-fiber composite, for example, the fibers are taken to have rectangular cross sections and the cross section of the RVE is a rectangle containing a square array of rectangular subcells.² In the simplest, four-subcell RVE, one subcell is a fiber cross section and the three others are matrix material (Fig. 1). This RVE is continuous and infinite along the fiber direction.

The MoC homogenization technique evolved out of a succession of research efforts by various workers. Sun, Achenbach, and Herrmann³ introduced the Effective Stiffness

Figure 1. Representative volume element for a continuous-fiber-reinforced composite.

Theory (EST) as an approximate technique for determining the macroscopic, dynamic elastic response of composite laminates. Their work introduced the notion that limited-order expansions for displacements within the subcells, which represent the unique material layers, provided a sufficient approximate solution for the dynamical response within an RVE for representing the effects of microstructure on the large-scale or long-wavelength deformation of a body or structure. EST was applied to calculating the dispersion behavior of elastic laminates.

Drumheller and Bedford applied the EST for determining dynamic displacements and stresses in elastic laminates.⁴ To calculate these additional dynamical variables, they introduced a number of extensions to the theory. They established the formalism for using higher-order expansions to describe the dynamical response within an RVE and extended the displacement continuity conditions in a consistent manner. They also introduced stress continuity conditions and expressed stress and displacement boundary conditions in a form compatible with the theory. They contributed to formalizing the explicit homogenization

process, also referred to as the "smoothing operation," by which the equivalent, homogeneous material model is generated from the detailed response of the RVE.

Aboudi developed the fundamentally important extension of the EST for treating inelastic response.⁵ This was achieved by introducing an approximation for the momentum conservation relation rather than generating the equations of motion from a Lagrangian action. The momentum conservation relation was converted to a hierarchy of relations for successive orders of subcell-averaged stress moments. Because the stress-moment equations derive from the general momentum conservation relation, arbitrary constitutive relations can be used for the component materials of the composite.

With this key extension, Aboudi and coworkers have applied his version of EST, renamed as the MoC, to two-phase composites configured as laminates, particulate inclusions in a matrix, and uni- or multidirectional, fiber-reinforced matrices with short, long, or random fibers.¹ The recent extension to more articulated RVEs in the Generalized Cells Method has enabled treatment of multiphase composites.² Application of the theory to fiber-reinforced composites was facilitated by treating idealized fibers having rectangular cross sections.⁶ This expedient was found to be a reasonable approximation provided the fiber cross-sectional area was preserved.^{6,7} By allowing retention of rectilinear RVEs, it permitted a straightforward extension of the technique as applied to laminates to continuous-fiber and short-fiber composites. The applications of the method include determinations of the following effective properties of equivalent, homogeneous continua: thermo-elastic constants; inelastic stress-strain curves; residual stresses and strains; initial and effective yield surfaces; imperfect interface bonding effects.¹ The MoC was developed for using an arbitrary order displacement expansion within each subcell.^{5,6} Microstructural dynamical effects do not enter the theory below the second-order approximation. The first-order version of the theory has been applied most widely. Its internal consistency and comparative ease of use make it versatile. This report is concerned only with application of the first-order theory. An outline for higher-order approximations will be given below as part of the general development of the theory.

Though the first-order theory represents explicitly only the macroscopic, quasi-static response of an RVE, this is often sufficient for applications with time resolution longer than wave transit times through characteristic structural dimensions and spatial resolution much larger than the microstructural dimensions. Many structural and material response problems meet these restrictions. However, difficulties develop in treating spatially averaged constitutive behavior of the pure constituents, such as progressive damage, that depends explicitly on strain localizations and stress concentrations.

Conceptual remarks concerning homogenization and the relation between the real, heterogeneous material and the equivalent, homogeneous-continuum model are presented next. The microstructural model used in the MoC is described in section III. Through the homogenization procedure, this leads to constitutive relations for an effective homogeneous continuum. These equations for the first-order version of the theory are collected in section IV. Macroscopic variables and the first-order theory continuum constitutive relations are discussed in section V. Section VI summarizes nonlinear elasticity theory and the method for introducing it into the first-order MoC homogenization procedure. Numerical procedures for implementing the rate-form MoC in a finite element method simulation are presented in section VII. Examples are given of nonlinear elasticity effects on the homogenized continuum response in section VIII. The report ends with a discussion in section IX.

II. REMARKS ON HOMOGENIZATION

The following remarks parallel Suquet's discussion of this topic.⁸ Two aspects are common to many homogenization techniques. First, the highly heterogeneous material is idealized as comprising a collection of identical RVEs that generate the whole material by periodic repetition. In random composites, the RVE is chosen as a statistically representative volume. In regular composites, like a continuous-fiber-reinforced matrix, which exhibit approximate periodicity, the RVE is the unit cell of the microstructure. In all cases the RVE is a useful idealization to the extent that it contains the dominant microstructural features and

the macroscopic response is not highly dependent on the aperiodicity of the microstructure. The choice of RVE produces fundamental differences among homogenization techniques. It can result in different macroscopic constitutive expressions even when the method of derivation of these laws is quite similar.⁸ As noted above, though the rectilinear RVE used in the MoC may appear to be a poor representation of fiber-reinforced composites, application of it demonstrates that it is not too deficient. Moreover, it is all-important to the theory in facilitating derivation of the overall-response description.

The second common feature is the use of separate coordinate systems: $\underline{y} \equiv \{y_i\}$ to describe the heterogeneous material and the RVE, and $\underline{x} \equiv \{x_i\}$ to describe the homogenized, macroscopic continuum. Microscopic variables, which describe the detailed state of the material within an RVE, are expressed as functions of $\underline{y}$ and time, t , and are parameterized in the continuum coordinates, $\underline{x}$. Examples are the stress and strain fields in an RVE: $\sigma_{ij}(\underline{y}, t; \underline{x})$ and $\epsilon_{ij}(\underline{y}, t; \underline{x})$, respectively. The parameterization in $\underline{x}$ results from the relation between the two coordinate systems: In the MoC technique, as well as in other homogenization techniques,⁸ an **entire** RVE maps into a **point** in the continuum coordinate system. Known macroscopic conditions at a continuum location provide boundary conditions for determining the thermomechanical state of the corresponding RVE through the governing equations. The complete state of the RVE, when mapped into the continuum, completes the determination of the macroscopic state at a given location.

III. MICROSTRUCTURAL MODEL

As is typical of homogenization techniques, the MoC assumes the behaviors of the constituent materials are known. Then, for the idealized microstructure, an approximate description is developed for the mechanical response of the RVE. Solution of the resulting equations completes determination of the dynamical variable values within each subcell. The macroscopic variable values are then obtained as volume averages of the subcell values.

The description of the RVE response for arbitrary order of approximation comprises three parts: truncated series expansions for every dynamical variable; application of subcell displacement and traction continuity conditions, on an average basis; moment expansion of the momentum conservation relation. The solution at a given time step provides the values of all the expansion coefficients for each dynamical variable.

Given an idealized RVE, such as that for a continuous-fiber-reinforced matrix shown in Fig. 1, the MoC homogenization technique begins by approximating the displacement field within each subcell with a truncated expansion in Legendre polynomials, P_m . Legendre polynomials simplify the analysis by being most convenient for expressing the boundary conditions for the chosen rectilinear RVE. For the N^{th} -order theory the displacement in subcell $(\alpha\gamma)$ of a continuous-fiber composite is represented as⁶

$$\underline{u}^{\alpha\gamma}(\underline{y}, t; \underline{x}) = \sum_{m,n=0}^N \underline{U}_{(mn)}^{\alpha\gamma}(\underline{x}, t) P_m(2y_2^\alpha/d_\alpha) P_n(2y_3^\gamma/h_\gamma), \text{ with } m+n < N+1 \quad (1)$$

Explicit summation is used in most equations to avoid confusion as to limits and which variables are summed. Even so, summation is always implied by repeated Latin indices, but never for Greek indices. Two-dimensional, local coordinate systems (y_2^α, y_3^γ) are defined within each subcell. The composite is periodic along the x_2 - and x_3 -directions. [Laminates and short-fiber composites are represented by a generalization of Eq. (1): Laminates are periodic in only the coordinate normal to the layering and a single Legendre series expansion is used; short fiber composites are periodic in all three coordinates and a triple Legendre series expansion is used.] Contrary to some early presentations,^{5,6} the expansions for stress and strain should always be truncated at the same order of approximation; namely $N-1$ with $m+n < N$. This guideline is consistent with more recent treatments⁹ and the earlier applications.⁶ The expansion coefficients $\underline{U}_{mn}^{\alpha\gamma}$ are the model microvariables whose values are sought. They determine the macroscopic stress in the effective homogenized continuum at the continuum location $\underline{x}$.

As with any approximate theory, it is of fundamental importance to maintain a consistent order of approximation. Accomplishing this first requires that "order" is clearly defined. Aboudi systematically omitted terms that involve factors $d_\alpha^p h_\gamma^q$ with $p + q > N$ because these were regarded as being of higher order of magnitude. The sum of the exponents does not indicate order of magnitude of such terms because d_α and h_γ are absolute quantities, not relative quantities like (d_α/D) and (h_γ/H) , where $D \equiv d_1 + d_2$ and $H \equiv h_1 + h_2$. Hence, it is inappropriate to omit any terms on the basis of the sum of exponents of the microstructural dimensions. Instead reference must be made to Eq. (1) to decide whether to retain a term. Legendre polynomials admit a useful characterization of their successive orders; the m^{th} order polynomial has m zero-crossings (nodes) and $(m - 1)$ extrema. A useful, and largely practical, expedient in determining the approximate mechanical response of the RVE is to limit our interest to the smoothest (i.e., least oscillating) contributions to the subcell displacement distribution. This corresponds to the polynomials with lowest index order. Orthogonality of the Legendre polynomials ensures that the coefficients for each order, $\underline{U}_{(mn)}^{\alpha\gamma}$ are independent of the number of terms retained in Eq. (1).

By this criterion, terms involving more than N nodes, i.e., $P_m P_n$ with $(m + n) > N$, should be omitted. This omission ensures that the subcell strain distribution, obtained from Eq. (1) using Eq. (3), includes terms having no more than $N-1$ nodes. The smoothest displacement contributions are not always the predominant ones, but the homogenization technique is useful only to the extent that these contributions dominate. Under quasi-static boundary conditions having spatial variations with a minimum wavelength that is large compared to the scale of the microstructure, the contribution to the displacement distribution in intact material decreases with decreasing smoothness.¹⁰ However, damage within any constituent produces some highly localized displacements, which correspond to significant contributions to the displacement from quite high order terms in Eq. (1). Under dynamic boundary conditions, even for those that vary slowly in space, the relative magnitudes of the different contributions to the displacement distribution depend on the applied loading frequency and the details of wave propagation within the composite. Generally, the

smoothness criterion will correspond to a magnitude criterion increasingly as the quotient of the wave speed in the composite and the loading frequency becomes much larger than the scale of the microstructure; e.g., the smallest subcell dimension.

From these considerations it should be understood that the MoC homogenization technique is of practical use only when displacement varies slowly on the microstructural scale. All of the derivations that follow assume this to be the case. In particular, the displacement is assumed to vary equally slowly along all three orthogonal directions, regardless of whether there is microstructure along the direction. This implies that higher-order spatial derivatives with respect to either local subcell coordinates (y) or macroscopic coordinates in the homogenized continuum (x) decrease in magnitude with increasing order.

Omitting terms on the basis of their smoothness provides a consistent order of approximation and has physically understandable consequences. Omitting terms on the basis of the sum of exponents of the microstructural dimensions, contrary to intention, does not preserve a consistent order of approximation, nor are its effects clear. Fortunately, these considerations do not affect the first-order theory, which is the main topic of this report.

The constitutive description assumes strain-rate superposition, elastically supported stresses, and a plasticity model. These are expressed as follows.

$$\dot{\epsilon}_{ij}^{\alpha\gamma} = \dot{e}_{ij}^{\alpha\gamma} + \dot{\eta}_{ij}^{\alpha\gamma}, \quad (2)$$

where e (η) denotes the elastic (plastic) strain and the dot denotes the time derivative. The small strain tensor is defined as

$$\epsilon_{ij}^{\alpha\gamma} = \frac{1}{2} \left[\frac{\partial u_i^{\alpha\gamma}}{\partial y_j} + \frac{\partial u_j^{\alpha\gamma}}{\partial y_i} \right], \quad (3)$$

with subcell coordinate y_i taken to be identical to x_i for the nonperiodic coordinates. Individual subcell rotations are neglected. The original theory adopted a linear stress-strain relation,^{5,6}

$$\sigma_{ij}^{\alpha\gamma}(y,t; \underline{x}) = C_{ijkl}^{\alpha\gamma} e_{kl}^{\alpha\gamma}(y,t; \underline{x}). \quad (4a)$$

$C_{ijkl}^{\alpha\gamma}$ are the second-order elastic constants (SOEC). Substituting a Legendre series expansion for stress, Eq. (A2), refer to Appendix A, and a similar one for elastic strain, then equating the coefficients of like powers of the spatial variables yields an analogous relation among the expansion coefficients:

$$\tau_{ij(m,n)}^{\alpha\gamma} = C_{ijkl}^{\alpha\gamma} \varepsilon_{kl(m,n)}^{\alpha\gamma}. \quad (4b)$$

The plastic strain rate can be determined from one of various plasticity models. Rate-dependent models are of particular interest. These may be described generally in terms of the Prandtl-Reuss flow rule

$$\dot{\eta}_{ij}^{\alpha\gamma} = \lambda_{\alpha\gamma} s_{ij}^{\alpha\gamma}, \quad (5)$$

where

$$\lambda_{\alpha\gamma}^2 = D_2^{\alpha\gamma} / J_2^{\alpha\gamma}. \quad (6)$$

s_{ij} denotes the subcell stress deviators and the flow function expression, Eq. (6), follows from Eq. (5) and the definitions of the stress deviator and plastic strain rate invariants

$$J_2^{\alpha\gamma} \equiv \frac{1}{2} s_{ij}^{\alpha\gamma} s_{ij}^{\alpha\gamma} \text{ and } D_2^{\alpha\gamma} \equiv \frac{1}{2} \dot{\eta}_{ij}^{\alpha\gamma} \dot{\eta}_{ij}^{\alpha\gamma}, \quad (7)$$

Different plasticity models correspond to different relations between J_2 and D_2 . The choice of flow function, $\lambda_{\alpha\gamma}$, is not constrained by the MoC theory.

Aboudi^{5,6} used the unified viscoplastic model developed by Bodner and Partom.¹¹ This flow model provides

$$D_2^{\alpha\gamma} = (D_o^{\alpha\gamma})^2 \exp \left[-\frac{n_{\alpha\gamma}+1}{n_{\alpha\gamma}} \left(\frac{Z_2^2}{3J_2^{\alpha\gamma}} \right)^{n_{\alpha\gamma}} \right], \quad (8)$$

and

$$Z_{\alpha\gamma} = Z_1^{\alpha\gamma} + (Z_o^{\alpha\gamma} - Z_1^{\alpha\gamma}) \exp[-m_{\alpha\gamma} w_p^{\alpha\gamma} / Z_o^{\alpha\gamma}], \quad (9)$$

where the plastic work rate is given by

$$\dot{w}_p^{\alpha\gamma} = 2 \lambda_{\alpha\gamma} J_2^{\alpha\gamma}. \quad (10)$$

The material constants of the flow model are n , m , Z_o , Z_1 , and D_o .^{6,11}

It is often convenient to use plasticity models with yield surfaces and associated flow as several calibrated models exist for representing the high strain rate response of metals. For such a flow model, beyond a certain stress level, J_2 is given as a function of D_2 and possibly other variables such as the second invariant of plastic strain, I_2 , and temperature, T . This function is the yield strength, Y , and the yield surface is given by

$$F \equiv \sqrt{J_2} - Y(D_2, I_2, T, \dots) = 0. \quad (11)$$

Applying the associated flow rule,

$$\dot{\eta}_{ij} \propto \frac{\partial F}{\partial \sigma_{ij}}, \quad (12)$$

to such a yield surface leads, again, to Prandtl-Reuss flow because here $\partial/\partial\sigma_{ij} = \partial/\partial s_{ij}$ and $\partial F/\partial s_{ij} = s_{ij} / \sqrt{J_2}$. The formal inverse of Eq. (11),

$$D_2 = Y^{-1}(J_2, I_2, T, \dots), \quad (13)$$

would be the analog of Eq. (8) for the particular plasticity model under consideration. D_2 is determined from this inverse function, or, more commonly, through an implicit solution procedure.

The theory for arbitrary order proceeds by expressing all dynamical variables as truncated Legendre expansions. In the first-order theory, the zero-order moment of the stress serves in place of the stress or its expansion coefficients. It is denoted as $S_{ij}^{\alpha\gamma}$ and is the volume-averaged stress in the $(\alpha\gamma)$ subcell where the averaging is per unit length along any continuous direction. Thus, for a laminate, it is the volume average stress per unit in-plane area; for a continuous-fiber composite, it is the volume average stress per unit length in the fiber direction. The relation between this zero-order stress moment and the stress expansion coefficients used in the higher-order theories is given in Appendix A. The zero- and first-order stress moments are proportional to the corresponding stress expansion coefficients.

The complete description of the approximate mechanical response of an RVE requires specification of subcell continuity conditions and derivation of approximate momentum conservation relations that are consistent with the order of truncated expansions for the subcell dynamical variables. We discuss the displacement and traction continuity conditions first, beginning with the former. Here, we explicitly treat the case of the **continuous-fiber composite** RVE shown in Fig. 1.

Accounting for the macroscopic variations that prevail around the continuum location $\underline{x}$ is of fundamental importance in developing the displacement continuity expressions. (Doing this is referred to as "the transition to the continuum."⁴⁻⁶) It introduces macroscopic strain information into the micromechanics, which ensures that the solution for the mechanical

response of the RVE is appropriate to the prevailing conditions at $\underline{x}$. In particular, the macroscopic displacement gradients provide boundary conditions on the approximate solution for the RVE response. Aboudi accounts for the macroscopic displacement variation with Taylor series in the continuum coordinates that are truncated at a consistent order of approximation.¹²

Displacement continuity begins from the exact conditions,

$$\underline{u}^{1\gamma}(y_2 = d_1/2, y_3, t; \underline{x}) = \underline{u}^{2\gamma}(y_2 = -d_2/2, y_3, t; \underline{x}), \quad (14a)$$

$$\underline{u}^{\alpha 1}(y_2, y_3 = h_1/2, t; \underline{x}) = \underline{u}^{\alpha 2}(y_2, y_3 = -h_2/2, t; \underline{x}), \quad (14b)$$

where perfect bonding between the constituents has been assumed. Substituting for $\underline{u}$ from Eq. (1) and evaluating $P_m(\pm 1) = (\pm 1)^m$ yields

$$\sum_{m,n=0}^N \underline{U}_{(mn)}^{1\gamma}(\underline{x}, t) P_n(2y_3^\gamma/h_\gamma) = \sum_{p,q=0}^N (-1)^p \underline{U}_{(pq)}^{2\gamma}(\underline{x}, t) P_q(2y_3^\gamma/h_\gamma), \quad (15a)$$

$$\sum_{m,n=0}^N \underline{U}_{(mn)}^{\alpha 1}(\underline{x}, t) P_m(2y_2^\alpha/d_\alpha) = \sum_{p,q=0}^N (-1)^q \underline{U}_{(pq)}^{\alpha 2}(\underline{x}, t) P_p(2y_2^\alpha/d_\alpha). \quad (15b)$$

These conditions cannot be satisfied identically along the respective subcell sides; i.e., for all y_3^γ in Eq. (15a) and for all y_2^α in Eq. (15b). Because ultimate interest is in the homogenized, macroscopic response, only an approximate description of the mechanical response of the RVE is sought. Hence, it is a reasonable expedient to require displacement continuity on average only.⁶ Averaging Eqs. (15a, b) over the respective free subcell coordinate reduces the displacement continuity conditions to

$$\sum_{m=0}^N \underline{U}_{(m0)}^{1\gamma}(\underline{x}, t) = \sum_{p=0}^N (-1)^p \underline{U}_{(p0)}^{2\gamma}(\underline{x}, t), \quad (16a)$$

$$\sum_{n=0}^N \underline{U}_{(0n)}^{\alpha 1}(\underline{x}, t) = \sum_{q=0}^N (-1)^q \underline{U}_{(0q)}^{\alpha 2}(\underline{x}, t). \quad (16b)$$

Following Aboudi,¹² approximate allowance is now made for the variation of $\underline{U}$ across the RVE at $\underline{x}$ by expanding $\underline{U}$ in a neighboring RVE in a Taylor series truncated at the order consistent with that of the rest of the description. This step in the development is well-founded conceptually, avoiding earlier allusions to macroscopic variations within an RVE.⁶ It will be sufficient to consider subcell interfaces parallel to y_3 . For the two adjacent RVEs the development leading to Eq. (16a) provides

$$\sum_{m=0}^N (-1)^m \underline{U}_{(m0)}^{1\gamma} = \sum_{p=0}^N \underline{U}_{(p0)}^{0\gamma}, \quad (17a)$$

$$\sum_{m=0}^N (-1)^m \underline{U}_{(m0)}^{3\gamma} = \sum_{p=0}^N \underline{U}_{(p0)}^{2\gamma}, \quad (17b)$$

where the independent variables are understood to be $(\underline{x}, t)$. The superscript (0γ) refers to the upper subcells in the lower adjacent RVE and superscript (3γ) refers to the lower subcells in the upper adjacent RVE. Taylor series to order N for the displacement coefficients in subcells (0γ) and (3γ) in terms of those in subcells (2γ) and (1γ) , respectively, are

$$\underline{U}_{(m0)}^{0\gamma} \approx \underline{U}_{(m0)}^{2\gamma} + \sum_{r=1}^{N-m} \frac{1}{r!} (-D)^r \frac{\partial^r}{\partial x_2^r} \underline{U}_{(m0)}^{2\gamma}, \quad (18a)$$

$$\underline{U}_{(m0)}^{3\gamma} \approx \underline{U}_{(m0)}^{1\gamma} + \sum_{r=1}^{N-m} \frac{1}{r!} D^r \frac{\partial^r}{\partial x_2^r} \underline{U}_{(m0)}^{1\gamma}. \quad (18b)$$

Substituting these expressions for the (0γ) and (3γ) subcell coefficients in Eqs. (17a, b) yields,

$$\sum_{m=0}^N (-1)^m \underline{U}_{(m0)}^{1\gamma} = \sum_{p=0}^N \left\{ \underline{U}_{(p0)}^{2\gamma} + \sum_{q=1}^{N-p} \frac{1}{q!} (-D)^q \frac{\partial^q}{\partial x_2^q} \underline{U}_{(p0)}^{2\gamma} \right\}, \quad (19a)$$

$$\sum_{m=0}^N (-1)^m \left\{ \underline{U}_{(m0)}^{1\gamma} + \sum_{n=1}^{N-m} \frac{1}{n!} D^n \frac{\partial^n}{\partial x_2^n} \underline{U}_{(m0)}^{1\gamma} \right\} = \sum_{p=0}^N \underline{U}_{(p0)}^{2\gamma}. \quad (19b)$$

Some manipulation of Eqs. (16a) and (19a, b) produces more convenient expressions for average displacement continuity. Subtracting Eq. (19b) from Eq. (19a) yields

$$-\sum_{m=0}^N (-1)^m \sum_{n=1}^{N-m} \frac{1}{n!} D^n \frac{\partial^n}{\partial x_2^n} \underline{U}_{(m0)}^{1\gamma} = \sum_{p=0}^N \sum_{q=1}^{N-p} \frac{1}{q!} (-D)^q \frac{\partial^q}{\partial x_2^q} \underline{U}_{(p0)}^{2\gamma}. \quad (20)$$

Subtracting Eq. (19b) from Eq. (16a) yields

$$\sum_{p=0}^{[(N-1)/2]} 2(\underline{U}_{(2p+1,0)}^{1\gamma} + \underline{U}_{(2p+1,0)}^{2\gamma}) = \sum_{m=0}^N (-1)^m \sum_{n=1}^{N-m} \frac{1}{n!} D^n \frac{\partial^n}{\partial x_2^n} \underline{U}_{(m0)}^{1\gamma}, \quad (21)$$

where [] in the upper limit denotes truncation to an integer value. Adding Eqs. (16a) and (19b) yields

$$\sum_{p=0}^{[N/2]} 2(\underline{U}_{(2p,0)}^{1\gamma} - \underline{U}_{(2p,0)}^{2\gamma}) = -\sum_{m=0}^N (-1)^m \sum_{n=1}^{N-m} \frac{1}{n!} D^n \frac{\partial^n}{\partial x_2^n} \underline{U}_{(m0)}^{1\gamma}. \quad (22)$$

Analogous equations apply to the interfaces parallel to y_2 :

$$-\sum_{m=0}^N (-1)^m \sum_{n=1}^{N-m} \frac{1}{n!} H^n \frac{\partial^n}{\partial x_3^n} \underline{U}_{(0m)}^{\alpha 1} = \sum_{p=0}^N \sum_{q=1}^{N-p} \frac{1}{q!} (-H)^q \frac{\partial^q}{\partial x_3^q} \underline{U}_{(0p)}^{\alpha 2}, \quad (23)$$

$$\sum_{p=0}^{[(N-1)/2]} 2(\underline{U}_{(0,2p+1)}^{\alpha 1} + \underline{U}_{(0,2p+1)}^{\alpha 2}) = \sum_{m=0}^N (-1)^m \sum_{n=1}^{N-m} \frac{1}{n!} H^n \frac{\partial^n}{\partial x_3^n} \underline{U}_{(0m)}^{\alpha 1}, \quad (24)$$

$$\sum_{p=0}^{[N/2]} 2(\underline{U}_{(0,2p)}^{\alpha 1} - \underline{U}_{(0,2p)}^{\alpha 2}) = - \sum_{m=0}^N (-1)^m \sum_{n=1}^{N-m} \frac{1}{n!} H^n \frac{\partial^n}{\partial x_3^n} \underline{U}_{(0m)}^{\alpha 1}. \quad (25)$$

Equations (20), (21), (22), and (23) should be used in place of Eqs. (13) through (14) of reference 6.

The exact traction continuity conditions are

$$\sigma_{2i}^{1\gamma}(y_2 = d_1/2, y_3, t; \underline{x}) = \sigma_{2i}^{2\gamma}(y_2 = -d_2/2, y_3, t; \underline{x}), \quad (26a)$$

$$\sigma_{2i}^{1\gamma}(y_2 = -d_1/2, y_3, t; \underline{x}) = \sigma_{2i}^{0\gamma}(y_2 = d_2/2, y_3, t; \underline{x}), \quad (26b)$$

$$\sigma_{3i}^{\alpha 1}(y_2, y_3 = h_1/2, t; \underline{x}) = \sigma_{3i}^{\alpha 2}(y_2, y_3 = -h_2/2, t; \underline{x}), \quad (26c)$$

$$\sigma_{3i}^{\alpha 1}(y_2, y_3 = -h_1/2, t; \underline{x}) = \sigma_{3i}^{\alpha 0}(y_2, y_3 = h_2/2, t; \underline{x}). \quad (26d)$$

As was done for displacement, the macroscopic variation in stress around the position $\underline{x}$ in the homogenized continuum is accounted for with a truncated Taylor series in the continuum coordinates,

$$\sigma_{2i}^{0\gamma}(y_2 = d_2/2, y_3, t; \underline{x}) = \sigma_{2i}^{2\gamma}(y_2 = d_2/2, y_3, t; \underline{x}) + \sum_{r=1}^{N-1} \frac{1}{r!} (-D)^r \frac{\partial^r}{\partial x_2^r} \sigma_{2i}^{2\gamma}. \quad (27)$$

Using Eq. (A2), refer to Appendix A, to represent stress and keeping a consistent order of approximation, this series becomes

$$\sigma_{2i}^{0\gamma}(y_2 = d_2/2, y_3, t; \underline{x}) = \sigma_{2i}^{2\gamma}(y_2 = d_2/2, y_3, t; \underline{x}) + \quad (28a)$$

$$\sum_{m,n=0}^{N-1} \sqrt{(1+2m)(1+2n)} P_n(2y_3^\gamma/h_\gamma) \sum_{r=1}^{N-1-(m+n)} \frac{1}{r!} (-D)^r \frac{\partial^r}{\partial x_2^r} (\tau_{2i(m,n)}^{2\gamma}).$$

Similarly,

$$\sigma_{3i}^{\alpha 0}(y_2, y_3 = h_2/2, t; \underline{x}) = \sigma_{3i}^{\alpha 2}(y_2, y_3 = -h_2/2, t; \underline{x}) + \sum_{m,n=0}^{N-1} \sqrt{(1+2m)(1+2n)} P_m(2y_2^\alpha/d_\alpha) \sum_{r=1}^{N-1-(m+n)} \frac{1}{r!} (-D)^r \frac{\partial^r}{\partial x_3^r} \left(\tau_{3i(m,n)}^{\alpha 2} \right). \quad (28b)$$

Equations (26) and (28) are used directly in the momentum conservation relation, as discussed next.

To maintain a consistent order of approximation in the description of the mechanical response of the RVE, the momentum conservation relation is expanded in a hierarchy of stress moment equations of motion. The series expansions are substituted for displacement and stress in this set of subcell-averaged stress-moment equations. In general, these are then solved numerically subject to appropriate displacement or stress boundary conditions .

To proceed, multiply the momentum conservation relation by $(y_2^\alpha)^p (y_3^\alpha)^q$ and average over a subcell,

$$\frac{1}{d_\alpha h_\gamma} \int_{-d_\alpha/2}^{d_\alpha/2} dy_2^\alpha (y_2^\alpha)^p \int_{-h_\gamma/2}^{h_\gamma/2} dy_3^\gamma (y_3^\gamma)^q \left\{ \partial_i \sigma_{ij}^{\alpha\gamma} = \rho_{\alpha\gamma} \ddot{u}_j^{\alpha\gamma} \right\}. \quad (29)$$

$\rho_{\alpha\gamma}$ is the density of the material in the $(\alpha\gamma)$ subcell. Integrating by parts and substituting the displacement and stress expansions yield the stress-moment equations of motion,⁶

$$\partial_1 S_{1j(p,q)}^{\alpha\gamma} + I_{2j(p,q)}^{\alpha\gamma} + J_{3j(p,q)}^{\alpha\gamma} - p S_{2j(p-1,q)}^{\alpha\gamma} - q S_{3j(p,q-1)}^{\alpha\gamma} = \rho_{\alpha\gamma} \left(\frac{d_\alpha}{2} \right)^p \left(\frac{h_\gamma}{2} \right)^q \sum_{m,n=0}^N \left\{ \ddot{u}_{j(m,n)}^{\alpha\gamma} c_m^p c_n^q / [(2m+1)(2n+1)] \right\}, \quad m+n < N+1 \quad (30)$$

where $p, q = 0, 1, \dots, N$ with $p + q < N + 1$. They are not summed. c_m^p are the Legendre series coefficients for z^p and $\partial_1 \equiv \partial / \partial x_1$. Equation (A1) in Appendix A defines the average stress moments $S_{ij(pq)}^{\alpha\gamma}$ analogously to Eq. (29), and

$$I_{2j(pq)}^{\alpha\gamma} \equiv \frac{1}{d_\alpha h_\gamma} \left(\frac{d_\alpha}{2} \right)^p \int_{-h_\gamma/2}^{h_\gamma/2} dy_3^\gamma (y_3^\gamma)^q \left\{ [\sigma_{2j}^{\alpha\gamma}]_{y_2^\alpha = d_\alpha/2} + (-1)^{p+1} [\sigma_{2j}^{\alpha\gamma}]_{y_2^\alpha = -d_\alpha/2} \right\}, \quad (31)$$

$$J_{3j(pq)}^{\alpha\gamma} \equiv \frac{1}{d_\alpha h_\gamma} \left(\frac{h_\gamma}{2} \right)^q \int_{-d_\alpha/2}^{d_\alpha/2} dy_2^\alpha (y_2^\alpha)^p \left\{ [\sigma_{3j}^{\alpha\gamma}]_{y_3^\gamma = h_\gamma/2} + (-1)^{q+1} [\sigma_{3j}^{\alpha\gamma}]_{y_3^\gamma = -h_\gamma/2} \right\}. \quad (32)$$

In these expressions the subscripted right bracket in Eqs. (31) and (32) denote the argument at which the stress is evaluated.

Substituting Eqs. (26) and (28) into Eqs. (31) and (32) yields the average traction continuity conditions:

$$I_{2j(pq)}^{1\gamma} = \left(-\frac{d_1}{d_2} \right)^{p-1} I_{2j(pq)}^{2\gamma} + \frac{2}{h_\gamma} \left(-\frac{d_1}{2} \right)^{p-1} \sum_{m,n=0}^{N-1} \sqrt{(1+2m)(1+2n)} \times \quad (33a)$$

$$\sum_{r=1}^{N-1-(m+n)} \frac{1}{r!} (-D)^r \frac{\partial^r}{\partial x_2^r} \left(\tau_{2j(m,n)}^{2\gamma} \right) \int_{-h_\gamma/2}^{h_\gamma/2} dy_3^\gamma (y_3^\gamma)^q P_n(2y_3^\gamma/h_\gamma),$$

and

$$J_{3j(pq)}^{\alpha 1} = \left(-\frac{h_1}{h_2} \right)^{q-1} J_{3j(pq)}^{\alpha 2} + \frac{2}{d_\alpha} \left(-\frac{h_1}{2} \right)^{q-1} \sum_{m,n=0}^{N-1} \sqrt{(1+2m)(1+2n)} \times \quad (33b)$$

$$\sum_{r=1}^{N-1-(m+n)} \frac{1}{r!} (-H)^r \frac{\partial^r}{\partial x_3^r} \left(\tau_{3j(m,n)}^{\alpha 2} \right) \int_{-d_\alpha/2}^{d_\alpha/2} dy_2^\alpha (y_2^\alpha)^p P_m(2y_2^\alpha/d_\alpha).$$

These relations should be used in place of Eq. (23) in reference 6. That these relations provide for traction continuity only on average over the side of a subcell is a consequence of the integrations contained in the definitions of the $I_{2j(pq)}^{\alpha\gamma}$ and $J_{3j(pq)}^{\alpha\gamma}$. Indeed, it is seen from these definitions that Eqs. (33a, b) actually express continuity of stress moments. Thus, traction continuity is applied on a different basis than is displacement continuity in the MoC homogenization technique. The relation between the order of terms in the Legendre series and the order of stress moments is ambiguous because for a given truncation of the Legendre series, stress moments, $S_{ij(p,q)}^{\alpha\gamma}$, and boundary integrals, $I_{2j(p,q)}^{\alpha\gamma}$ and $J_{3j(p,q)}^{\alpha\gamma}$, of arbitrary order (p, q) can be computed [see Eqs. (A3) and (B3), Appendices A and B]. The constraint $p + q < N + 1$ in Eq. (30) results from requiring that the set of stress moment equations is consistent (see discussion in Appendix B).

Equations (33a, b) are combined with the displacement continuity conditions, Eqs. (20), (21), (22), and (23), the constitutive relations, Eqs. (2), (4), and (5), the stress-moment equations, Eqs. (28a and b), and initial and boundary conditions to obtain a determinate set of equations that is solved for the microvariables, and subsequently the stress in the equivalent homogenized continuum.⁵ For illustration, in Appendix B Eq. (30) is expanded for the case $N = 2$. There it is seen that dynamic effects do not contribute to the microstructural response unless a second- or higher-order treatment is performed.

A recent modification of the first-order MoC generalizes the rectilinear RVE to an arbitrary number of subcells.² The elaborated RVE is useful for better representing actual packing configurations of the fiber reinforcement. Though the displacement field within this RVE is approximated by a multiply piecewise-linear function, the generalized method does not constitute a higher-order theory. This is evident from consideration of the stress field within the elaborated RVE. Owing to traction continuity, along the x_2 -direction, say, for each γ the $S_{2j}^{\alpha\gamma}$ will be equal for all α . Indeed, the $S_{23}^{\alpha\gamma}$ components of subcell stress are uniform throughout the RVE, regardless of the number of subcells.

IV. FIRST-ORDER THEORY EXPRESSIONS

The developments and applications in the remainder of this report pertain to the first-order theory specifically. For convenience, expressions for the variables and the governing conditions for the first-order, rate-form description are given here.

The particle velocity is given by the time derivative of Eq. (1) with $N = 1$,

$$\dot{u}_i^{\alpha\gamma}(\underline{y}, t; \underline{x}) = \dot{w}_i^{\alpha\gamma}(\underline{x}, t) + \dot{\phi}_i^{\alpha\gamma}(\underline{x}, t) y_2^\alpha + \dot{\psi}_i^{\alpha\gamma}(\underline{x}, t) y_3^\gamma. \quad (34a)$$

To simplify the algebra, the coefficients $U_{i(mn)}^{\alpha\gamma}$ have been replaced with:

$$w_i^{\alpha\gamma} \equiv U_{i(00)}^{\alpha\gamma} ; \phi_i^{\alpha\gamma} \equiv \frac{2}{d_\alpha} U_{i(10)}^{\alpha\gamma} ; \psi_i^{\alpha\gamma} \equiv \frac{2}{h_\gamma} U_{i(01)}^{\alpha\gamma} . \quad (34b)$$

The time derivative of Eq. (3) then leads to rates of deformation¹³ that are spatially uniform within each subcell,

$$\dot{\epsilon}_{ij}^{\alpha\gamma} = \frac{1}{2} \left[\frac{\partial \dot{u}_i^{\alpha\gamma}}{\partial y_j} + \frac{\partial \dot{u}_j^{\alpha\gamma}}{\partial y_i} \right]. \quad (35)$$

Substituting from Eq. (34a) the individual strain rates are found to be

$$\begin{aligned} \dot{\epsilon}_{11}^{\alpha\gamma} &= \dot{\bar{\epsilon}}_{11} = \dot{\bar{w}}_{1,1} ; \dot{\epsilon}_{22}^{\alpha\gamma} = \dot{\phi}_2^{\alpha\gamma} ; \\ \dot{\epsilon}_{33}^{\alpha\gamma} &= \dot{\psi}_3^{\alpha\gamma} ; 2\dot{\epsilon}_{23}^{\alpha\gamma} = \dot{\phi}_3^{\alpha\gamma} + \dot{\psi}_2^{\alpha\gamma} ; \\ 2\dot{\epsilon}_{13}^{\alpha\gamma} &= \dot{\bar{w}}_{3,1} + \dot{\psi}_1^{\alpha\gamma} ; 2\dot{\epsilon}_{12}^{\alpha\gamma} = \dot{\bar{w}}_{2,1} + \dot{\phi}_1^{\alpha\gamma} . \end{aligned} \quad (36)$$

Equations (39a), (40a), and (41) were used in writing the $\dot{\epsilon}_{ij}$ components; the overbar denotes macroscopic quantities. The subscripted comma denotes differentiation with

respect to the $\underline{x}$ -component identified by the index following it. Consistent with these, the stresses too are uniform within each subcell. This is denoted by replacing $\sigma_{ij}^{\alpha\gamma}$ in the constitutive relations [Eqs. (4) and (5)] by $S_{ij}^{\alpha\gamma}$, the zero-order stress moment, Eq. (A1) in

Appendix A:

$$S_{ij}^{\alpha\gamma}(\underline{y}, t; \underline{x}) = C_{ijkl}^{\alpha\gamma} e_{kl}^{\alpha\gamma}(\underline{y}, t; \underline{x}) ; \quad (37)$$

$$\dot{\eta}_{ij}^{\alpha\gamma} = \Lambda_{\alpha\gamma} s_{ij}^{\alpha\gamma}. \quad (38)$$

Here, the elastic and plastic strains are uniform within each subcell, $s_{ij}^{\alpha\gamma}$ now denotes the deviator of $S_{ij}^{\alpha\gamma}$, and $\Lambda_{\alpha\gamma}$ are the subcell-average values of $\lambda_{\alpha\gamma}$. The latter are the leading terms of the Legendre series expansions of the $\lambda_{\alpha\gamma}$. Strain-rate superposition still holds between the uniform subcell values shown in Eq. (2),

$$\dot{\epsilon}_{ij}^{\alpha\gamma} = \dot{e}_{ij}^{\alpha\gamma} + \dot{\eta}_{ij}^{\alpha\gamma}.$$

For a first-order treatment ($N = 1$) using Eq. (10), Eqs. (20) through (22) become

$$\dot{w}_{i,2}^{1\gamma} = \dot{w}_{i,2}^{2\gamma} \equiv \dot{w}_{i,2}^{\gamma} ; \quad (39a)$$

$$d_1 \dot{\phi}_i^{1\gamma} + d_2 \dot{\phi}_i^{2\gamma} = D \dot{w}_{i,2}^{\gamma} ; \quad (39b)$$

$$\dot{w}_i^{2\gamma} = \dot{w}_i^{1\gamma} + \frac{D}{2} \dot{w}_{i,2}^{\gamma} . \quad (39c)$$

Similarly, Eqs. (23) through (25) become

$$\dot{w}_{i,3}^{\alpha 1} = \dot{w}_{i,3}^{\alpha 2} \equiv \dot{w}_{i,3}^{\alpha} ; \quad (40a)$$

$$h_1 \dot{\psi}_j^{\alpha 1} + h_2 \dot{\psi}_j^{\alpha 2} = H \dot{w}_{j,3}^{\alpha} ; \quad (40b)$$

$$\dot{w}_i^{\alpha 2} = \dot{w}_i^{\alpha 1} + \frac{H}{2} \dot{w}_{i,3}^{\alpha} . \quad (40c)$$

These conditions are augmented by asserting equality of all the subcell velocity gradients with the respective macroscopic gradients, denoted by overbars:

$$\dot{\bar{w}}_{i,2}^{\gamma} = \dot{\bar{w}}_{i,2} ; \quad \dot{\bar{w}}_{i,3}^{\alpha} = \dot{\bar{w}}_{i,3} . \quad (41)$$

This assumption is standard in the solution procedure,^{1,2,6,12} but seems overly restrictive. This paragraph considers relaxing this assumption in the (x_2, x_3) plane. Subtracting Eq. (40c) with $\alpha = 1$ from the $\alpha = 2$ equation and using Eq. (39c) to identify velocity gradient terms lead to a relation among the gradients,

$$D (\dot{w}_{i,2}^{\gamma=2} - \dot{w}_{i,2}^{\gamma=1}) = H (\dot{w}_{i,3}^{\alpha=2} - \dot{w}_{i,3}^{\alpha=1}) . \quad (42)$$

Referring to Eqs. (39c) and (40c), this relation is seen to express the equality of the mixed second derivatives of displacement. Rather than adopting Eq. (41), assume that the velocity gradients are volume averages of the subcell values,

$$\dot{\bar{w}}_{i,j} \equiv \frac{1}{DH} \sum_{\alpha,\gamma=1}^2 d_{\alpha} h_{\gamma} \dot{w}_{i,j}^{\alpha\gamma} . \quad (43)$$

The value of defining macroscopic quantities as volume averages is discussed in the next section. The additional value of Eq. (43) is that, in combination with Eqs. (39a,b) and (40a,b), it implies that the macroscopic strain is given by the volume average of the subcell strains and is related to the macroscopic displacements $\underline{w}$ according to the small strain definition. Equation (43) provides two vector relations for the gradients in the (x_2, x_3) plane:

$$H \dot{\bar{w}}_{i,2} = h_1 \dot{w}_{i,2}^{\gamma=1} + h_2 \dot{w}_{i,2}^{\gamma=2} , \quad (44a)$$

$$D \dot{\bar{w}}_{i,3} = d_1 \dot{w}_{i,3}^{\alpha=1} + d_2 \dot{w}_{i,3}^{\alpha=2} . \quad (44b)$$

A less restrictive treatment of the gradients in the (x_2, x_3) plane would become possible upon specifying one vector relation among the gradients $\dot{w}_{i,2}$ and $\dot{w}_{i,3}$ in addition to Eqs. (42) and (44). Such a treatment would introduce a new degree of freedom into the subcell strains. This change would affect the microvariable values obtained as approximate solutions for the mechanical response and, consequently, also affect the overall response. We have not been successful in identifying or devising the desired relation.

Equations (39c) and (40c) also serve to demonstrate that setting all the $\dot{w}^{\alpha\gamma}$ equal to the macroscopic displacement at $\underline{x}$ is not consistent with average displacement continuity. Although this was the stated procedure in previous work,^{1,2,6,12} the error was of no consequence because the subcell displacements do not enter into the model solution. The procedure actually used was to adopt Eq. (41).

As illustrated in Appendix B, in the first-order treatment traction continuity Eqs. (33a, b) reduce to one pair of relations, Eqs. (B7a) and (B8b), which are given here using Eq. (A3) in Appendix A, and putting the result in rate form

$$\dot{S}_{2j}^{1\gamma} = \dot{S}_{2j}^{2\gamma} , \quad (45a)$$

$$\dot{S}_{3j}^{\alpha 1} = \dot{S}_{3j}^{\alpha 2} . \quad (45b)$$

The MoC, as described by the preceding equations, is suitable for use as the material model in a numerical continuum mechanics (CM) computer program with explicit time integration. The CM program determines the strain rates of a computational element and passes this information to the material subroutine. Hence, in this application the composite model response needs to be solved for conditions of a steady, uniformly applied macroscopic strain rate, $\dot{\epsilon}_{ij}$. Ideally, the solution consists of values of the 24 microvariables, $\dot{\phi}_i^{\alpha\gamma}$ and $\dot{\psi}_i^{\alpha\gamma}$. These quantities and the plastic strain rates, $\dot{\eta}_{ij}^{\alpha\gamma}$, fully determine the subcell stresses and strains through Eqs. (36), (37), and (2). As described in

the next section, the macroscopic stresses in the computational element, $\bar{\sigma}_{ij}$, are then obtained from volume averages of the subcell stresses. These volume-averaged stress values, which constitute the response of an equivalent homogeneous continuum, are returned to the CM program and computation proceeds to the next computational element.

For the case of steady, uniformly applied macroscopic strain rates, all nine of the velocity gradient components are known. The continuity conditions provide one equation too few to determine all 24 microvariables explicitly. Displacement continuity Eqs. (39b) and (40b) provide 12 equations, but traction continuity, Eqs. (45a,b), provide only 11 equations because the stress tensor is symmetric; only three of the relations involving $S_{23}^{\alpha\gamma}$ are independent. Because the microvariables $\dot{\phi}_3^{\alpha\gamma}$ and $\dot{\psi}_2^{\alpha\gamma}$ occur only as a sum [see Eq. (36)], a solution can be obtained for 20 microvariables⁹: $\dot{\phi}_i^{\alpha\gamma}$, $i = 1, 2$; $\dot{\psi}_j^{\alpha\gamma}$, $j = 1, 3$; $\dot{\zeta}^{\alpha\gamma} \equiv \dot{\phi}_3^{\alpha\gamma} + \dot{\psi}_2^{\alpha\gamma}$. A displacement continuity relation for the $\dot{\zeta}^{\alpha\gamma}$ is obtained by setting $\gamma = \alpha$, multiplying Eq. (39b) by h_α , and adding Eq. (40b) multiplied by d_α . Adding the two relations obtained for the two values of α yields

$$d_1 h_1 \dot{\zeta}^{11} + d_2 h_1 \dot{\zeta}^{21} + d_1 h_2 \dot{\zeta}^{12} + d_2 h_2 \dot{\zeta}^{22} = 2DH \dot{\epsilon}_{23}. \quad (46)$$

Equations (39b) with $i = 1, 2$, (40b) with $j = 1, 3$, and (46) are nine displacement conditions, which together with 11 independent traction conditions, Eqs. (45a, b), form a determinate set of equations from which the 20 microvariable values can be determined. In an explicit time integration calculation, the plastic strain rates are adequately determined using stress values from the preceding time step.

V. MACROSCOPIC CONTINUUM RELATIONS

For the MOC, the stress and strain at a point in the equivalent, homogenized continuum are given by the RVE volume average of the corresponding subcell quantities whose values were determined subject to the macroscopic conditions at the continuum

location. (The volume average is per unit length along any continuous directions. See section III.) For continuous-fiber composites the volume average per unit length along the fiber is

$$\bar{f}_{ij} \equiv \frac{1}{DH} \sum_{\alpha, \gamma=1}^2 d_{\alpha} h_{\gamma} f_{ij}^{\alpha\gamma}, \quad (47)$$

where f represents stress, strain (total, elastic or plastic), or strain rate, and the overbar denotes the macroscopic value of the quantity. This definition has a number of appealing properties. First, it provides a macroscopic total strain that is related to the macroscopic displacements according to the small strain definition.⁶ Second, it is the analog for the case of piecewise constant fields within the RVE of the volume average considered by Hill.¹⁰ Defining macroscopic stress and strain in this way and defining the macroscopic elastic constants as the proportionality between them, Hill demonstrated that the macroscopic stress (strain) is fully determined by the tractions (displacements) on the surface of the RVE. Furthermore, for boundary conditions on the composite that would produce homogeneous stress or strain in a homogeneous body, the volume-averaged strain energy equals one half of the product of the macroscopic stress times the macroscopic strain. For a first order CM calculation the strain on a computational element is uniform and so this result applies. However, Hill's results rely on the following conditions. When these are not fulfilled, the properties of the macroscopic quantities just described no longer obtain exactly: The body is under static equilibrium with no internal stresses; there are no body forces; the elastic compliances are bounded (no voids); the sample is macroscopically homogeneous.

For the case of applied macroscopic strain, Aboudi found that, for anisotropic elastic or isotropic elastic-plastic constituents, the model solution described in the previous section could be cast as a tensor expression for the macroscopic stress in terms of the macroscopic strain plus terms linear in the subcell plastic strain components.⁹ The

practical value of this macroscopic constitutive relation is the determination of analytic expressions for the effective elastic constants of continuous-fiber-reinforced composites whose constituents possess at least transversely isotropic symmetry. The macroscopic symmetry of the composite is found to be orthorhombic, having nine unique elastic constants, in general. Corresponding to this symmetry, the 20 equations in the determinate set decouple into 8 that determine the normal stresses and 4 each that determine the shear stresses individually.⁹

In an explicit time integration calculation, the formal macroscopic constitutive relation is of little practical use because computation of the plastic strains requires solving for the microvariables at each time step. Once the values of the microvariables are known, the macroscopic stress is easily obtained from Eq. (47). The macroscopic constitutive relation may be of greater use in time-implicit calculations.

Some care is needed in using the reported expressions for the effective elastic constants⁹ as they contain typographical errors. In particular, the denominator D in Eq. (22) of reference 9 should be omitted. They duplicate the D factor given in the definitions in the appendix. Also, note that some expressions can be simplified by explicitly writing each $v_{\alpha\gamma}$ as $d_{\alpha}h_{\gamma}$ and canceling terms. For example, Q_1 given in the appendix of reference 9 reduces to $Q_1 = v_{11}(T_1 + T_9) \times (C_{12}^f C_{12}^m)$.

It is also of interest to solve the composite model for the case of applied macroscopic stress rate. This solution permits calculation of the overall hydrostatic response of the anisotropic composite, for example. The solution is obtained simply by augmenting the determinate set of equations from the applied macroscopic strain rate case by the six relations from Eq. (47) that define the macroscopic stress rates. The macroscopic strain rates are the six additional unknowns; the velocity gradient matrix is symmetric because the solution is given in the RVE coordinate frame.

VI. NONLINEAR ELASTICITY

A. Detailed Treatment

Stress states with a high mean stress often occur under dynamic loading. Mean stresses in the range of 10s to 100s of MPa can produce significant deviations from the linear stress-elastic strain relation, Eq. (4), depending on the particular stress configuration and on the composite. To adequately simulate this aspect of the dynamic response of composites to the high strain-rate loadings typical of crash-safety, armor, and munitions applications, we extended Eq. (4) to include the terms that are quadratic in elastic strain within the framework of the first-order MoC homogenization procedure. This extension modifies the calculated response throughout the deformation. Its effects are not limited to the strain interval of purely elastic response because even during inelastic deformation the stress depends on only the elastic contribution to the total strain. The quadratic terms, which represent the leading order of nonlinearity in the stress-elastic strain relation, are determined from the thermodynamic definition for higher-order elastic constants and the relation between Cauchy and Piola-Kirchoff stress measures.

Following Brugger's definition for n^{th} order isentropic (isothermal) elastic constants as the n^{th} order derivative of internal (Helmholtz) energy with respect to elastic Lagrangian finite strain, E ,¹⁴ the second Piola-Kirchoff stress, T_{ij} , can be represented as a Taylor series in strain measured from the stress-free state,¹⁵

$$T_{ij}(E, z) = C_{ijkl}^z E_{kl}^e + \frac{1}{2} C_{ijklmn}^z E_{kl}^e E_{mn}^e + \dots \quad (48)$$

Here the C_{ijkl} (C_{ijklmn}) are the second (third) order elastic constants [SOEC (TOEC)] and z denotes temperature or entropy, as appropriate to the application. Cauchy stress in terms of the second Piola-Kirchoff stress is given by,¹⁵

$$\sigma_{ij} = \frac{\rho}{\rho_0} \frac{\partial x_i}{\partial X_k} \frac{\partial x_j}{\partial X_n} T_{kn} \quad , \quad (49)$$

where ρ (ρ_0) is (initial) density and the partial derivatives are the deformation gradients.¹³ Substituting for T_{ij} in Eq. (49) from Eq. (48) truncated after the terms quadratic in strain and substituting strain expansions for the relative density and displacement gradients,¹⁵

$$\frac{\rho}{\rho_0} \approx 1 - E_{kk} \quad \text{and} \quad \frac{\partial x_i}{\partial X_j} \approx \delta_{ij} + E_{ij} - \frac{1}{2} E_{ki} E_{kj}, \quad (50a,b)$$

yields¹⁵

$$\begin{aligned} \sigma_{ij} \approx & C_{ijkl} E_{kl}^e + C_{ipkl} E_{kl}^e E_{jp}^e + C_{ipkl} E_{kl}^e E_{ip}^e \\ & - C_{ijkl} E_{kl}^e E_{pp}^e + \frac{1}{2} C_{ijklmn} E_{kl}^e E_{mn}^e, \end{aligned} \quad (51)$$

where the superscript z has been suppressed. In the material reference frame, Lagrangian strain in terms of small strain is given by,¹⁵

$$E_{ij}^e = e_{ij} + \frac{1}{2} e_{ki} e_{kj}. \quad (52)$$

Substituting for E_{ij} in Eqs. (50a, b) and retaining terms to only second order in small strain yields the desired extension of Eq. (4),

$$\begin{aligned} \sigma_{ij} \approx & C_{ijkl} (e_{kl} + \frac{1}{2} e_{pk} e_{pl}) + C_{ipkl} e_{kl} e_{jp} + C_{pjkl} e_{kl} e_{ip} \\ & - C_{ijkl} e_{kl} e_{pp} + \frac{1}{2} C_{ijklmn} e_{kl} e_{mn}. \end{aligned} \quad (53)$$

In Appendix C this equation is expanded for the case of orthorhombic symmetry. The quadratic expressions for the nonlinear subcell stress components in the first-order MoC theory are also given there. Brugger's table of third-order elastic constants (TOEC) was helpful for expanding Eq. (53).¹⁶

To implement Eq. (53) in the MoC procedure, we assume orthorhombic (orthotropic) symmetry for the constituents. This symmetry was convenient because the 29 SOECs and TOECs are unique except for the usual Voigt symmetry.¹⁵ This uniqueness facilitated systematic manipulations when writing out the traction continuity conditions, Eqs. (45), with the subcell stress components given by Eqs. (C9) through (C14) in Appendix C. Additionally, orthorhombic symmetry is a useful choice as several symmetry classes of interest are obtained as special cases: isotropic, cubic, hexagonal (transversely isotropic), some tetragonal classes.^{14,17}

A non-rate form, numerical solution procedure for the first-order MoC theory with the nonlinear constitutive relation, Eq. (53), replacing Eq. (4), was implemented in a one-cell program called FONE (First-Order Nonlinear Elasticity). FONE is described in Appendix D. From Eqs. (2) and (36) it is seen that the elastic strain nonlinearity of Eq. (53) corresponds to the same order of nonlinearity in the microvariables whose values are sought. This makes it necessary to solve the traction continuity conditions iteratively. The program provides the overall mechanical response of uniformly loaded, unidirectional, continuous-fiber composites for conditions of applied macroscopic strain or applied macroscopic stress. The former solution provides a check on solutions in rate-form obtained in the material model subroutine of a continuum mechanics computer program [see discussion in section VII]. The applied stress solution was pursued as a guide for generating an efficient, but accurate, alternative to the full tensor solution for applied strain conditions. This is discussed further in the second part of this section.

For both boundary conditions, iterative solutions are obtained by a Newton-Raphson method using microvariable values determined with the linear stress-elastic strain relation, Eq. (4), as the seed values. For applied macroscopic strain conditions, these seed values are used to evaluate eleven subcell traction continuity conditions, as before [see discussion of Eq. (44)], but with the subcell stresses given by the quadratic elastic strain expressions, Eqs. (C9) through (C14). Corrections to the eleven microvariable values, $\Delta\varphi$, are obtained

simultaneously by multiplication of the inverse partial derivative matrix, $\underline{\underline{P}}^{-1}$, and the traction discontinuities, $\underline{\chi}$:

$$\underline{\chi} \approx \underline{\underline{P}} \cdot \Delta \underline{\phi} \rightarrow \underline{\underline{P}}_{ij}^{-1} \chi_j \approx \Delta \phi_i. \quad (54)$$

Here, $\underline{\underline{P}}_{ij} \equiv \nabla_i^\phi \chi_j$,

$$\underline{\chi} \equiv (S_{22}^{11} - S_{22}^{21}, S_{22}^{12} - S_{22}^{22}, S_{33}^{11} - S_{33}^{12}, S_{33}^{21} - S_{33}^{22}, S_{23}^{11} - S_{23}^{21},$$

$$S_{23}^{12} - S_{23}^{22}, S_{23}^{21} - S_{23}^{22}, S_{13}^{11} - S_{13}^{12}, S_{13}^{21} - S_{13}^{22}, S_{12}^{11} - S_{12}^{21}, S_{12}^{12} - S_{12}^{22}),$$

$$\underline{\phi} \equiv (\phi_1^{11}, \phi_2^{11}, \phi_1^{22}, \phi_2^{22}, \psi_1^{11}, \psi_3^{11}, \psi_1^{22}, \psi_3^{22}, \zeta^{11}, \zeta^{21}, \zeta^{22}),$$

$\Delta \underline{\phi}$ is the corresponding vector of corrections, and ∇_i^ϕ denotes partial differentiation with respect to these eleven microvariables. The microvariable values are improved by evaluating $\underline{\chi}$ and $\underline{\underline{P}}$ with the n^{th} set of values and calculating the n^{th} corrections from Eq. (54). Adding these corrections to the n^{th} set of microvariable values yields the $(n + 1)^{\text{st}}$ set of values. This iteration scheme is continued until a suitable numerical convergence is achieved. We take the solution to be converged when the relative corrections are all less than 100 ppm in absolute value.

Unlike the solutions obtained when the linear elasticity relation is used,^{9,18} analytic macroscopic stress/macroscopic strain expressions cannot be obtained when quadratic elasticity is used. This is because the nine macroscopic displacement gradients occur individually in the quadratic stress continuity expressions; they cannot be collectively replaced by the six strain components. The macroscopic stress of the homogenized continuum must be computed explicitly from the converged microvariable values using Eq. (47) with $\bar{f}^{\alpha\gamma} = S^{\alpha\gamma}$ and $\bar{\mathbf{f}} = \bar{\boldsymbol{\sigma}}$. Hence, the applied strain boundary condition requires specification of all nine macroscopic displacement gradients. This presents no difficulty, as the nine values are available upon entering the material model routine in a continuum

mechanics computer program. Additionally, the freedom to assign the displacement gradients individually facilitates specification of pure or simple shear in, e.g., one-cell simulations.

Our experience is that, in strain ranges of interest, converged solutions are obtained in less than ten iterations. The converged stress values can differ from the initial linear estimates by more than 20%, but most of this difference is from the nonlinear strain terms. The converged microvariable values differ from the seed values by only a few per cent.

For applied macroscopic stress boundary conditions, the eleven quadratic stress continuity equations are augmented by six macroscopic stress definitions, Eq. (47), and the macroscopic strain are six additional unknowns. (Because these equations are solved in the RVE reference frame, the macroscopic displacement gradient matrix is symmetric and fully determined by the six macroscopic strains.) With these additions, numerical solutions are obtained in a manner similar to that for applied strain conditions. The augmented version of Eq. (54) is

$$\underline{\kappa} \approx \underline{Q} \cdot \Delta \underline{v} \rightarrow Q_{ij}^{-1} \kappa_j \approx \Delta v_i \quad . \quad (55)$$

$\underline{\kappa}$ is $\underline{\chi}$ augmented by the differences of each applied macroscopic stress component and the stress value calculated from the microvariable values from the previously completed iteration [subscript (n - 1)]:

$$\underline{\kappa} \equiv (\chi_i, \bar{\sigma}_1 - \bar{\sigma}_{1(n-1)}, \bar{\sigma}_2 - \bar{\sigma}_{2(n-1)}, \bar{\sigma}_3 - \bar{\sigma}_{3(n-1)}, \\ \bar{\sigma}_4 - \bar{\sigma}_{4(n-1)}, \bar{\sigma}_5 - \bar{\sigma}_{5(n-1)}, \bar{\sigma}_6 - \bar{\sigma}_{6(n-1)}) \quad . \quad (56)$$

The matrix of partial derivatives is $Q_{ij} \equiv \nabla_i^v \kappa_j$, the vector of unknowns is $\underline{v} = (\varphi_i, i = 1, 11; \bar{\epsilon}_k, k = 1, 6)$, $\Delta \underline{v}$ is the corresponding vector of corrections, and ∇_i^v denotes partial

differentiation with respect to these 17 variables. Tensor index pairs are abbreviated using conventional Voigt notation¹⁷: (11, 22, 33, 23, 13, 12) $\rightarrow$ (1, 2, 3, 4, 5, 6) with $\bar{\epsilon}_4 = 2\bar{\epsilon}_{23}$, $\bar{\epsilon}_5 = 2\bar{\epsilon}_{13}$, and $\bar{\epsilon}_6 = 2\bar{\epsilon}_{12}$.

These solution procedures were tested for pure isotropic materials under uniaxial strain and hydrostatic loading, for which analytic solutions can be determined. Stress-strain paths calculated with FONE by putting 6061-T6 aluminum into all four subcells reproduce the analytic results for these two loadings. Figure 2 illustrates the contributions from nonlinear elasticity to the uniaxial strain response of 6061-T6 aluminum. This material was chosen because of the availability of values for the elastic constants.¹⁹ For illustration purposes, the inelastic response was described by Eqs. (5) through (10) in which the parameter values for 2024-T4 aluminum²⁰ were used. The applied strain rate was below the sensitivity of the Bodner-Partom flow model.

Figure 2. Uniaxial strain of 6061-T6 aluminum.

In Fig. 2, volumetric strain equals the applied uniaxial strain, which is given on the abscissa. The component of stress in the direction of the uniaxial strain, referred to as the "longitudinal" stress, is given on the ordinate. The solid line is the response including nonlinear elasticity, Eq. (51). The dashed line is the response computed using linear elasticity, Eq. (4). Hugoniot data (peak states for uniaxial strain impact loading) for two aluminum alloys are given by the symbols.²¹ For both calculations, yielding is noticeable as the break in the curve near 0.5% strain. The chosen flow model involves little hardening and, after yielding occurs, the longitudinal stress response closely parallels the hydrostat, as expected. Including nonlinear elasticity effects is seen to produce much better agreement with the data. In particular, nonlinear elasticity makes substantial and increasing contributions after yielding has occurred. This is to be expected because the loading is purely a volumetric compression. Two contributions to the remaining discrepancy between the data and calculation are evident. First, only the leading order elastic nonlinearity was included. Higher-order nonlinear contributions may be significant in the data. Second, the calculation is purely mechanical. Temperature changes that accompany the dynamic compression were not taken into account. Each of these phenomena would tend to steepen the calculated response.

The ratio of the finite measure of uniaxial strain to the small strain measure is 1.050 at 10% strain. This suggests that inaccuracy in the small strain measure used in this non-rate-form application of the MoC model may also contribute to the remaining discrepancy. However, this does not account for the gross disagreement between the data and the response calculated assuming linear elasticity (dashed line). An explicit nonlinear dependence on the strain measure is required to achieve the substantial agreement with data shown in Fig. 2.

In rate-form, the MoC equations including nonlinear elasticity can be integrated explicitly. This would be a simpler method than the iterative, non-rate-form solution given by Eq. (54). Expressing the 11 independent rate-form traction continuity equations, Eqs. (45a and b), in terms of the microvariables using time derivatives of Eqs. (C9) through (C14) in Appendix C entails products of microvariables and their time derivatives.

Only the latter are unknown quantities in an explicit solution procedure and these terms occur linearly. Using values of the microvariables and elastic constants from the previous time step, the increment in microvariables can be computed by solving the simultaneous system of 11 linear equations. This solution method is compatible with the rate-form MoC equations, rate-dependent plasticity, as well as damage that is represented by degraded elastic constants.

An alternative representation for nonlinear elasticity may be desirable when progressive damage that requires updating the SOEC values for each time step is included in the homogenization procedure. By collecting terms, Eqs. (C3) through (C8) can be formally expressed as linear in the strain components with strain-dependent SOECs. For example, Eq. (C3) becomes

$$\dot{\alpha}_1 = C_{11}^* \dot{e}_1 + C_{12}^* \dot{e}_2 + C_{13}^* \dot{e}_3 + C_{14}^* \dot{e}_4 + C_{15}^* \dot{e}_5 + C_{16}^* \dot{e}_6, \quad (57)$$

where

$$C_{11}^* \equiv C_{11} + \frac{1}{2} [e_1 (C_{111} + 3C_{11}) + e_2 (C_{112} - C_{11} + C_{12}) + e_3 (C_{113} - C_{11} + C_{13})], \quad (58a)$$

$$C_{12}^* \equiv C_{12} + \frac{1}{2} [e_2 (C_{122} - C_{12}) + e_1 (C_{112} - C_{11} + C_{12}) + e_3 (C_{123} - C_{12} - C_{13})], \quad (58b)$$

$$C_{13}^* \equiv C_{13} + \frac{1}{2} [e_3 (C_{133} - C_{13}) + e_1 (C_{113} - C_{11} + C_{13}) + e_2 (C_{123} - C_{12} - C_{13})], \quad (58c)$$

$$C_{14}^* \equiv \frac{1}{8} e_4 (4C_{144} + C_{12} + C_{13}), \quad (58d)$$

$$C_{15}^* \equiv \frac{1}{8} e_5 (4C_{155} + C_{11} + C_{13} + 8C_{55}), \text{ and} \quad (58e)$$

$$C_{16}^* \equiv \frac{1}{8} e_6 (4C_{166} + C_{11} + C_{12} + 8C_{66}) . \quad (58f)$$

Using such formally linear expressions, the solution procedure for rate-form MoC equations with linear elasticity can be followed with the addition that the elastic constants in each subcell are updated to reflect both the current elastic strain according to relations like Eqs. (58a through f) and, possibly, the current state of damage, also. The simplification of treating equations that are formally linear is gained at the expense of having to regard all materials as having triclinic symmetry. This requires rederiving the MoC equations for the case of linear elasticity with no symmetry in the SOEC tensor.

B. Approximate Treatment

Here, we consider approximate constitutive relations for the pure constituents that have sufficient accuracy to include all significant phenomena that can result from elastic nonlinearity and anisotropy. Our purpose in this is to develop a robust and efficient numerical algorithm and to mitigate the common lack of complete sets of TOECs for the constituents.

An approximate treatment of nonlinearity in isotropic constituents is well-known and widely used^{22,23}: Because shear stress is limited by material strength, the predominant contribution of nonlinear elasticity is through volumetric strain. In isotropic materials the volumetric strain affects only the mean stress. Consequently, the mean and deviatoric stresses can be computed independently of one another. Elastic nonlinearity is approximately and accurately accounted for by computing the mean stress from an equation of state (EOS), with the stress deviator obtained from Equations (5), (6), and (11) with a chosen plasticity model.

Use of a microstructural description, such as the MoC homogenization technique, makes it possible to apply this EOS approximation to the common composite configuration of strong, anisotropic, brittle fibers in an isotropic, ductile matrix. The fibers are treated as

anisotropic, linear elastic up to failure. In each matrix subcell, the mean stress is described by a volume- and energy-dependent EOS, with the deviatoric stress given by a rate-dependent plasticity model. The equation of state provides a convenient means of accounting for the common increase of the matrix material bulk modulus with compression. This is the predominant nonlinear elasticity contribution for this important configuration of composite. It makes it possible for shock waves to develop in the material and, for this reason, is an essential aspect of the constitutive response. The details of this approximation for graphite reinforced epoxy are given in the next section.

In an anisotropic constituent material, volumetric strain again makes the predominant contribution to nonlinear elasticity. However, in general the volumetric and deviatoric responses are coupled. Nonetheless, in the absence of post-yield hardening (or softening), any changes in the deviatoric stress components are small and the deviatoric stress invariant is constant. Hence, the post-yield mean stress/volumetric strain response should nearly parallel the hydrostat if the hardening is small. When it is, the EOS approximation may be applicable to the post-yield response of anisotropic constituents.

It is instructive to consider the applied-stress response of an anisotropic constituent to better understand when the EOS approximation may be applicable. Application of hydrostatic pressure produces deviatoric strain, which changes the sample shape, while application of deviatoric stress can change the volumetric strain. Because the magnitude of deviatoric stress is bounded by material strength, it can produce only limited volumetric strain. At large mean stress values, this is likely to be a negligible contribution to volumetric strain. (At low mean stress, it can be a significant contribution.) The shape changes resulting from applied mean stress are not similarly limited.

In a composite, the deformation of each constituent is constrained by that of the others. The coupling between volumetric and deviatoric response in anisotropic constituents can influence the overall response of a composite through the displacement and traction continuity conditions on internal interfaces between different constituent materials. The EOS approximation can be inadequate for describing anisotropic

constituents for this reason. Two additions to the EOS approximation are needed for it to be applicable to anisotropic constituent materials. First, the effects of shape changes should be included. Second, the strain path dependence (i.e., dependence on the full strain state) of the mean stress/volumetric strain curve of each anisotropic constituent needs to be evaluated. The contribution from elastic nonlinearity is often not important before yielding and after yielding the mean stress/volumetric strain curve deviates from the paralleling the hydrostat due to hardening. Hence estimates of the deviations due to hardening are needed for each anisotropic constituent to accurately approximate the post-yield mean stress.

Provided values for the TOECs are available, the one-cell program simulations of the response of a composite of interest are useful for evaluating whether the EOS approximation, which is more efficient, is sufficiently accurate. Duplicate one-cell simulations are made for a variety of load paths including both applied strain and applied stress. One simulation of each pair uses the detailed constitutive model involving SOECs and TOECs, while the second simulation uses a candidate approximate constitutive model. The agreement of the computed response between each pair of simulations is indicative of the adequacy of the approximate constitutive relation.

VII. COMPUTATIONAL PROCEDURES

The first-order MoC in rate form with imperfect bonding¹² was implemented as a material model for graphite fiber reinforced epoxy in a one-dimensional (1-D) CM program generalized to treat anisotropy. This material model uses the approximate treatment of elastic nonlinearity for isotropic constituents, described above. With this material model, the 1-D program is suitable for simulating the overall thermomechanical response of structures that are partially or fully composed of a unidirectional composite of strong, brittle fibers in an isotropic matrix. The rate-form MoC equations were also implemented in the three-dimensional CM program EPIC²⁴ and used to simulate the response of graphite fiber reinforced aluminum. For each computational element ("cell"),

both programs provide the material model subroutine with internal energy and velocity gradients: deformation rates and rotation rates. In this rate-form implementation of the MoC model, the deformation rates are the strain rates and there is no restriction to small strain. Because the MoC equations are most easily expressed in the reference frame of the composite, the current rotations are used to transform the strain rates into this frame.²⁵ The plastic strain rates are updated according to Eqs. (5) through (10) and the MoC rate-equations are solved. In the present application, the spin matrix serves as an adequate approximation to the angular velocity matrix in transforming from the cell to RVE coordinate frames.²⁶ Finally, the macroscopic stress state of the element is computed from Eq. (47) with $\mathbf{f}^{\alpha\gamma} = \mathbf{S}^{\alpha\gamma}$ and $\bar{\mathbf{f}} = \bar{\boldsymbol{\sigma}}$, and it is transformed back into the cell reference frame.

In the MoC equations, the mean stress in each epoxy matrix subcell is represented by a Mie-Grüneisen expression,

$$-\frac{1}{3} S_{kk}^{\alpha\gamma} = H(\epsilon)(1 - \Gamma\epsilon/2) + \rho \Gamma E. \quad (59)$$

Here, the volumetric strain $\epsilon = 1 - v_0/v$, Γ is the Grüneisen constant, E is isothermal internal energy change from an initial unstressed state. This expression follows from integrating the identity $\rho\Gamma = (\partial P/\partial E)_v$ with $\rho\Gamma$ constant, and using the Rankine-Hugoniot energy jump condition to relate the energy of the dynamically stressed material to pressure, P , and volume.²² In Eq. (59) we assume a linear relation between the uniaxial shock wave velocity (U_s) and the particle velocity (U_p)

$$U_s = c + s U_p, \quad (60)$$

with

$$H(\epsilon) = \frac{\rho_0 c^2 \epsilon(\epsilon-1)}{(1 + \epsilon(s-1))^2}. \quad (61)$$

This representation was chosen because many epoxies display a linear U_s - U_p behavior.²¹ To facilitate the implementation of the equation-of-state into the numerical algorithm, a

cubic polynomial approximation was used for the Hugoniot, $H(\epsilon)$. With this choice, for each matrix subcell Eq. (59) becomes

$$-\frac{1}{3} S_{kk} = a_1 \mu + a_2 \mu^2 + a_3 \mu^3 + a_4 \mu^4 + (b_0 + b_1 \mu) E, \quad (62)$$

where

$$\begin{aligned} a_1 &= -\rho_0 c^2, \\ a_2 &= \rho_0 c^2 (2s - 1 - \frac{1}{2} \Gamma), \\ a_3 &= -\rho_0 c^2 [3s^2 - 4s + 1 - \frac{1}{2} (2s - 1) \Gamma], \\ a_4 &= \rho_0 c^2 [4s^3 - 9s^2 - 2s + 1 - \frac{1}{2} (3s^2 - 4s + 1) \Gamma], \\ b_0 &= \rho_0 \Gamma, \\ b_1 &= -\rho_0 \Gamma. \end{aligned}$$

By applying displacement continuity Eqs. (39b) and (40b), and traction continuity Eqs. (45a, b), the solution to the MoC equations is programmed as four simultaneous linear equations for the normal stress microvariables and analytic expressions for each of the shear stress microvariables⁹ (see Appendix E). Hence, the only extraordinary computation required is inversion of a 4×4 coefficient matrix. Because the matrix elements depend on the SOECs, the inverse must be computed whenever the SOECs change during a simulation to represent nonlinear elasticity through strain-dependent constants or degradation due to damage.

A plasticity model with a yield surface was used with the elastically nonlinear, rate-form MoC model in EPIC to simulate a metal matrix composite subjected to high strain-rate loading.²⁷ The phenomenological Johnson-Cook plasticity model²⁸ was used because it has the form common to many, physically based, high strain-rate yield models that are calibrated for metals, like the Mechanical Threshold Stress (MTS) model.²⁹ The plastic strain rates are determined as follows when such a plasticity model is used in conjunction with the MoC homogenization technique. Trial subcell deviatoric stress component values are obtained by augmenting the previous time step values by the respective elastic predictions. Next, these trial deviatoric stress component values for the matrix subcells are

tested against the yield condition. If $\sqrt{J_2}$ exceeds the current value of the yield function, Y , the stress deviators are each reduced in proportion $Y/\sqrt{J_2}$. The corrected matrix subcell stress deviator values then provide the current plastic strain rate values through Eqs. (2) and (4):

$${}_n\dot{\eta}_{ij}^{\alpha\gamma} = {}_n\dot{\epsilon}_{ij}^{\alpha\gamma} - \frac{1}{2G\Delta t} ({}_n s_{ij}^{\alpha\gamma} - {}_{n-1} s_{ij}^{\alpha\gamma}), \quad i \neq j, \quad (63)$$

where the pre-subscripts refer to the time step and G is the isotropic matrix shear modulus. The stress calculation is completed by again solving the MoC rate equations, but now with the plastic strain rate values obtained from Eq. (63). The step is completed by computing the macroscopic stress state of the element and transforming it back into the cell coordinate frame.

As currently implemented, the final stress deviator values for the matrix subcells satisfy the yield condition only approximately. This error has been ignored. It may be possible to compute this second solution of the MoC rate equations subject to the constraint that the stress deviators remain on the yield surface. This would be desirable and needs to be pursued. The second MoC computation, after determining the plastic strain rates, is unnecessary for the present application to the epoxy matrix composite because the viscoplasticity model allows direct determination of the plastic strain rates. Each computation of the MoC solution requires approximately 17% more time than calculating the response of an elastic, perfectly plastic material.

Damage models for the constituent materials can be easily included when they can be solved explicitly. In this case, the final microvariable values obtained from solving the MoC rate-equations are used to test whether the subcell stresses cause additional damage within any constituent. Damage effects can be represented by modifying the elastic constant values. The values for each subcell need to be updated each time step to represent progressive damage. (This leads to different elastic constant values in subcells containing

the same material.) Using these degraded elastic constant values in the MoC rate equations in the subsequent time step couples material damage into the stress determination.

VIII. EXAMPLES

In this section the nonlinear elasticity treatments are applied to calculating the mechanical response of two unidirectional fiber-reinforced composites. First, the detailed treatment is applied in a simulation of the response of T-50 Graphite fiber-reinforced 6061 T-6 aluminum (Gr/Al) to uniform uniaxial strain and hydrostatic loadings. This example illustrates potentially large contributions from nonlinear elasticity even at low strains. Following this, the EOS approximation, described above, is applied to a graphite-fiber-reinforced epoxy (Gr/E). After calibrating the model for pure epoxy to standard test data at a range of strain rates, the implementation of the rate-form MoC model, just presented, is found to produce good agreement with measured high rate uniaxial strain response of the Gr/E composite.

In composites, the constituent materials might not experience greater strain than 2% because substantial interfacial damage develops. Figure 2 demonstrates that, in pure aluminum, linear elasticity is sufficient below about 2% strain. However, within a composite the nonlinear elasticity contributions can be significant at low strain. This is illustrated in Fig. 3, which shows the overall response to uniaxial strain loading transverse to the fibers of graphite-fiber-reinforced aluminum (Gr /Al) computed with the one-cell program. The fibers are taken to have square cross sections and occupy 30% of the volume. The fibers lie along the x_1 -direction and the uniaxial strain is applied along the x_3 -direction; the $\bar{\sigma}_{33}$ stress component is the longitudinal stress. The solid lines are the normal stresses computed when nonlinear elasticity is included. The dashed lines are the normal stresses computed using linear elasticity. The heavy, short-dashed line is the longitudinal stress in pure aluminum from Fig. 2. In this

Figure 3. Calculated uniaxial strain response of Gr/Al composite transverse to the fibers.

calculation, the aluminum is treated as in Fig. 2. The graphite is treated as anisotropic, linearly elastic with no yield or failure. The elastic constants were determined from modulus values²⁰ and are given in Table 1. In Table 1 the material X_1 axis is taken to parallel the fiber axis and tensor index pairs are abbreviated using conventional Voigt notation¹⁷:

$$(11, 22, 33, 23, 13, 12) \rightarrow (1, 2, 3, 4, 5, 6) \text{ with } e_4 \equiv 2e_{23}, e_5 \equiv 2e_{13}, \text{ and } e_6 \equiv 2e_{12}.$$

The large transverse compliance of graphite fibers causes the longitudinal stress response in the Gr/Al composite to fall below that of the pure aluminum. Also, stress concentrations produced by the inhomogeneity of the composite cause yielding to occur at a lower macroscopic strain than in the pure aluminum. As in pure aluminum, the nonlinear elasticity effects are substantial, particularly after yielding: Using linear elasticity underestimates the longitudinal stress by about 25% at 1.5% strain and it fails to exhibit the correct qualitative behavior of the transverse normal stress components. The post-yield

response is understandable in reference to the response of pure aluminum. The stress components dominated by the aluminum matrix, the σ_{33} and σ_{22} components, approximately parallel the hydrostat for aluminum, which is the expected

Table 1. Material properties used in simulations.

	6061-T6 Al	Epoxy	T-50 Graphite ^b	IM7 Graphite
C_{11} (GPa)	109.6 ^a	8.07 ^c	392.90	265.80
C_{22} (GPa)	109.6 ^a	8.07 ^c	9.61	11.10
C_{23} (GPa)	54.4 ^a	4.39 ^c	4.37	0.08
C_{13} (GPa)	54.4 ^a	4.39 ^c	5.73	4.59
C_{66} (GPa)	27.6 ^a	1.84 ^c	14.90	14.90
C_{111} (GPa)	-1408.0 ^a			
C_{112} (GPa)	-280.0 ^a			
C_{123} (GPa)	-185.0 ^a			
D_o (ms ⁻¹)	10.0 ^b	1750.00	0.00	
n	10.0 ^b	1.09	1.00	
m	300.0 ^b	1.00	1.00	
Z_o (GPa)	0.34 ^b	0.415	1.00	
Z_1 (GPa)	0.435 ^b	0.420	1.00	
^a Reference 16.				
^b Reference 17.				
^c Reference 30.				

behavior. The transverse normal stress in the fiber direction, the σ_{11} component, is a mixture of the aluminum and graphite constituents' responses; it falls in between paralleling the aluminum hydrostat and following the linear graphite response. Differences in the TOECs in the aluminum and graphite lead to the crossing of the two transverse normal stress curves. In particular, the strict linearity of the graphite response and the nonlinearity in the mean stress response of the aluminum produce the crossing here.

We emphasize that substantial contributions from elastic nonlinearity occur in this composite at strains below 2%. Strains of this magnitude are within the range of interest in high strain-rate applications like armor and crash response. Such strains are likely to produce damage, which was omitted from the calculation and will certainly strongly affect the composite response. Nonetheless, the large magnitude of the elastic nonlinearity effect suggests that it can make significant contributions to the overall composite response even in the presence of damage. Furthermore, the ratio of the finite uniaxial strain to the small strain measure used in this non-rate-form calculation is only 1.010 at 2% strain, making finite strain effects largely negligible.

For reference, Fig. 4 shows the overall mean stress/volumetric strain response of the Gr/Al composite. The mean stress under the uniaxial strain loading of Fig. 3 is shown by the dot-dashed line and that under hydrostatic loading is given by the solid line. Yielding is marked by the abrupt slope changes in each of these curves. Yielding occurs under hydrostatic loading because the material heterogeneity gives rise to stress concentrations. For comparison, the dashed line is purely elastic hydrostatic response; plasticity was suppressed in the calculation. The difference in the mean stress/volumetric strain response for different loading paths before yielding results from nonlinear elasticity. It occurs generally, even in homogeneous samples and for any material symmetry including isotropy. The magnitude of this load-path dependence for a given material symmetry is determined by the SOEC and TOEC values. In homogeneous materials with no hardening,

Figure 4. Calculated mean stress/volumetric strain relations for Gr/Al composite.

the post-yield mean stress curves for different load paths would parallel the hydrostat. Here, there is negligible hardening in the aluminum but the curve for uniaxial strain loading does not parallel the curve for hydrostatic loading. Like the occurrence of yielding under hydrostatic loading, this lack of parallelism also arises from the heterogeneity of the composite. The detailed shape of the post-yield curves is controlled by the homogenization model, and so is subject to experimental verification.

Next, we apply the approximate treatment of nonlinear elasticity effects as presented under Computational Procedures to the Gr/E composite. The epoxy model was calibrated with the following information. The density, ultrasonic longitudinal wave speed of 2.52 km/s and shear wave speed of 1.203 km/s in the epoxy³⁰ provide the SOEC values given in Table 1. The uncertainty in these wave speeds is approximately 5%. In Table 2, c

corresponds to the bulk wave speed ($\sqrt{K/\rho}$), where K is the epoxy bulk modulus. Due to lack of data, the s value for EPON 828 epoxy²² and the Grüneisen parameter value for polymethylmethacrylate (PMMA)³¹ were used for the present epoxy and the s value was fit as described below. The rate-dependent, uniaxial stress response of the epoxy versus true strain, represented by the Bodner-Partom plasticity model parameters in Table 1, are shown by the solid lines in Fig. 5. These parameters were determined by fitting the data given in this figure with the elastic response specified by the moduli obtained from the ultrasonic wave speeds. The solid symbols are the uniaxial tensile stress response measured at strain rates of 10^{-4} s^{-1} and 1 s^{-1} .³² These stress data have been corrected for changes in cross-sectional area. The dashed lines are results from two equivalent Hopkinson bar tests³³ at 3000 s^{-1} strain rate.³⁴ The Bodner-Partom model was motivated by dislocation dynamics. This model is chosen for the epoxy, based on comparisons with the experimental data for a wide range of strain-rates. A nearly linear unloading response was observed experimentally for the epoxy for small time scales. The fit shown in Fig. 5 is nonunique and was not optimized in any objective manner. Alternate sets of values of the plasticity model

Table 2. Equation of state parameters used in simulations.

	Epoxy	z-cut Quartz ^d	PMMA
$\rho \text{ (g/cm}^3\text{)}$	1.27 ± 0.005^a	2.65	1.184 ^e
$c \text{ (km/s)}$	2.103 ^a	6.36	2.76 ^e
s	1.543 ^b	1.36	1.4264 ^e
Γ	1.0 ^c	0.653	1.0 ^c
^a Reference 30 ^b Reference 21 ^c Reference 24 ^d Reference 26 ^e Reference 27

Figure 5. Fit of viscoplasticity model (solid lines) to data for epoxy.

parameters give qualitatively equivalent fits to this data but lead to substantially different responses when extrapolated to the higher strain rates occurring in shock wave experiments.

The value of s from Eq. (60) was chosen by simulating a shock wave experiment on the pure epoxy. The resulting fully-constrained epoxy constitutive model was used in one-dimensional simulations of shock wave experiments on the epoxy and the Gr/E composite. In experiments by Hixson,³⁰ dynamic uniaxial strain was produced in each target by parallel plate impact of a compound plate of z-cut quartz³⁵ backed by PMMA.³⁶ A schematic of the impact configurations is shown in Fig. 6. Table 2 gives the parameters used to model the impactor materials and Table 3 gives the details of the impact configurations. The dense set of points in Fig. 7 gives the measured free surface velocity history for the epoxy target. Time is given relative to the shock wave arrival. The solid

line is the simulated response for the epoxy which includes the nonlinear elasticity effects produced with $s = 2.2$ (Table 2). Two other simulation results are shown for comparison. The dashed curve is the response for the same s value, but with no plastic deformation. The dot-dashed curve is the response for linear elasticity ($b_1 = 0$ and $a_i = 0$ for $i > 1$ in Eq. [42]) combined with plasticity, as usual. These results illustrate that plastic deformation lowers the peak free-surface velocity and increases the rise times of both the loading and unloading waves. The predominant effects of the elastic nonlinearity are to increase the shock wave speed and to counter the increase in rise time of the loading wave caused by plasticity. Increasing s also reduces the peak free-surface velocity.

Increasing s beyond 2.2 improves the agreement of the solid curve with the observed loading wave rise time but further reduces the calculated peak free-surface velocity. This peak amplitude would be raised by enhancing the strain rate dependence of the plasticity model, which would reduce the amount of plastic deformation in the simulation. Hence, improving the agreement of the simulated and observed responses requires better constraining both the high strain-rate plasticity response and s , which characterizes the elastic nonlinearity. Two shock wave experiments on the epoxy in which wave speed and

Figure 6. Schematic of parallel plate impact configuration.

Table 3. Plate impact experiments and simulations.

Target Material	Thickness (mm)		Impact Velocity (km/s)	Calculated Peak Stress (GPa)
	z-cut Quartz/PMMA	Sample/Window		
Epoxy	2.57/5.0 ^a	2.78/0.0 ^a	0.500 ^a	1.46
Graphite/Epoxy	90° 1.557/5.0 ^a	2.807/5.0 ^a	0.496 ^a	1.70
Graphite/Epoxy	45° 4.0/2.0	3.0/4.0	0.5	2.31

^aReference 30

Figure 7. Measured and simulated response of epoxy to plate impact loading.

particle velocity are measured could suffice for directly determining s from Eq. (60). With s determined, the correct strain rate dependence would be obtained by choosing the plasticity parameters to simultaneously reproduce both the low- and moderate-rate uniaxial stress data of Fig. 5 and the high rate, uniaxial strain data of Fig. 7. Because we lack an objective means of separating the nonlinear elasticity from the strain rate-dependent plasticity effects, we use the parameter values at hand for illustration.

Similar one-dimensional simulations were performed to compare with an experiment performed on the unidirectional Gr/E composite shocked across the fibers. This experiment used the VISAR technique³⁶ to measure the velocity history of the interface of the composite sample with a transparent interferometry window of PMMA.³⁰ The measured interface velocity is shown by the dense set of points in Fig. 8, which are plotted relative to the shock wave arrival time. The oscillations about the peak amplitude are a common feature of the dynamic response of fiber-reinforced composites. The oscillatory response is suggestive of dispersion in linear elastic periodic structures. This supports the prevalent interpretation that these oscillations result from transient stress wave interactions in the microstructure of the inhomogeneous material.

The simulation of this experiment was performed using the fully-constrained epoxy model for the three matrix subcells of the RVE and a linear elastic-fiber model in the fourth subcell. The fibers and RVE were both taken to have square cross sections. The fiber volume fraction was 0.58. The elastic properties of the IM7 graphite fibers were partially determined from the ultrasonic longitudinal wave speeds in the composite.³⁰ The speeds parallel and transverse to the fibers were 10.155 ± 0.406 km/s and 2.855 ± 0.143 km/s, respectively. The composite density was 1.56 ± 0.01 g/cm³.³⁰ These values were used to determine the axial and transverse Young's moduli by assuming the shear modulus and Poisson's ratios equaled those of T-50 graphite fiber.²⁰ The effective elastic constants of the composite that were used to match the measured wave speeds were computed from the MoC model.⁹ This procedure yielded a fiber axial Young's modulus of 263 GPa and a transverse Young's modulus of 15 GPa. The corresponding fiber SOECs

are given in Table 1. Notice that this determination differs substantially from simple mixture theory. This is evident, for example, when the latter is used to try to recover the longitudinal wave speed in the composite transverse to the fibers from the C_{22} values of Table 1, which yields 2.510 km/s rather than 2.855 km/s.

In Fig. 8a, the simulation result using the complete epoxy model for the matrix subcells is given by the solid curve; the result when plasticity is suppressed is given by the dashed curve; the result for linear elasticity is given by the dot-dashed curve. There is fair agreement between the simulation with the complete epoxy model and the observed interface velocity amplitude and release wave arrival times. As in Fig. 7, comparing the solid and dot-dashed curves demonstrates that the elastic nonlinearity makes a substantial contribution to the material response. It is apparent that enhancing the strain rate dependence of the plasticity would further improve the agreement. The observed oscillations are completely absent from the simulations because the first order MoC model uses a static solution to momentum conservation within the RVE. As a result, all dynamic response on the time scale of wave propagation through the RVE is suppressed.

The actual configuration of the fibers in the composite is not well represented by the chosen RVE. The composite is built up from fibers collected into tows. Tows are formed into a tape and tapes are laid up with epoxy. Despite these details in the composite construction, the MoC model gives reasonable results. Figure 8b illustrates qualitative effects of fiber aspect ratio. Lacking detailed images of the composite microstructure, we have no basis for choosing the appropriate fiber aspect ratio for the comparison with plate impact data. We define aspect ratio as the dimension along the wave propagation direction over the dimension transverse to the propagation direction. The initial portion of the wave from Fig. 8a that was computed using the complete epoxy model is again shown by the solid line, but here plotted versus time from impact. The two broken curves were generated by repeating the wave calculation using the same constitutive models for the fiber and epoxy, but changing the fiber aspect ratio from unity to 2/3 (dashed line) and 3/2 (dot-dashed line), successively. The RVE aspect ratio was unity for all three calculations.

Figure 8a. Simulation of a plate impact experiment on Gr/E loaded transverse to the fibers. Comparison of data (dots) with calculations including elastic nonlinearity and plasticity (solid), elastic nonlinearity, only (dashed), and linear elasticity and plasticity (dot-dashed).

Figure 8b. Simulation of a plate impact experiment on Gr/E loaded transverse to the fibers. Comparison of fiber aspect ratio effects.

The differences evident in Fig. 8b have identifiable causes. The dashed line shows that a smaller fraction of fiber thickness along the propagation direction leads to a slower compression wave speed than for the square fiber cross-section calculation (solid line). This is consistent with the epoxy having lower wave speeds than the fiber. Based on the discussion of Fig. 8a, the higher amplitude of the dashed curve indicates that less plastic strain occurs. Even so, the mean stress in the epoxy must be higher than for the square fiber case to account for the earlier arrival of the unloading wave. This is an effect of the elastic nonlinearity of the epoxy matrix. Without it the unloading wave for this case would arrive after that for the square fiber and the compression wave arrival would be even later than seen in the figure.

The compression wave in the composite with fiber aspect ratio $3/2$ (dot-dashed curve) arrives much sooner than that for the square fiber case due to the larger fraction of fiber thickness along the wave propagation direction. The higher amplitude seen for this case also indicates that less plastic strain occurs. Unlike the composite with fiber aspect ratio $2/3$, the later arrival of the unloading wave shows that the lower plastic strain is not accompanied by higher mean stress.

Finally, Fig. 9 shows additional effects of the composite anisotropy upon uniaxial strain wave propagation. For purposes of this illustration, the simulation presented in Fig. 8 was replicated with the fiber orientation changed to be inclined 45° to the impact plane rather than 90° . For this orientation the impact produces two plane waves, one quasi-longitudinal and one quasi-transverse.³⁷ The interface velocity that would be produced by these waves in the nonlinear elastic composite with plasticity suppressed is shown by the dashed lines in Fig. 9a plotted against time from impact. This result is helpful to interpreting the complicated response. Fig. 9b shows the interface velocity produced by the same impact using the complete epoxy model for the matrix subcells of the composite.

For the 45° orientation, both waves make contributions to v_1 , the particle velocity in the wave propagation direction. The quasi-longitudinal wave arrives first, making a

Figure 9a. Calculated mixed-mode waves in Gr/E impacted at 45° to the fiber direction. Result with no plasticity is shown.

Figure 9b. Calculated mixed-mode waves in Gr/E impacted at 45° to the fiber direction. Result with complete epoxy model for the matrix subcells.

positive contribution to v_1 and a negative contribution to v_2 , the transverse particle velocity in the plane of the fibers. This wave travels at 7.3 km/s, which is faster than the pure longitudinal wave from the 90° orientation (2.9 km/s) because its speed is augmented by the axial response of the graphite fibers. The v_1 and v_2 amplitudes both increase at 1.2 μ s when the quasi-transverse wave arrives. This raises the longitudinal interface velocity to its peak value. The release wave arriving at 1.6 μ s is identified as a quasi-longitudinal wave because the changes in v_1 and v_2 are again of opposite sign. This wave is produced by the wave reflected from the quartz/PMMA interface within the impactor when it impinges on the quartz/sample interface. The quasi-transverse wave produced by this same interaction at the quartz/sample interface arrives later than the times shown. Two quasi-transverse release waves arrive at 1.95 μ s and 2.4 μ s. These are generated by multiple reflections and mode conversion within the sample.

IX. DISCUSSION AND CONCLUSIONS

The preceding example illustrates the importance of properly treating anisotropy in CM computer programs in order to correctly simulate the variety of response it can produce. A proper treatment requires the entire stress tensor, as well as all three components of the vector momentum conservation relation, even in one-dimensional calculations. In one-dimensional calculations, three strain components can be nonzero.

Micromechanics-based models, such as the MoC model, are advantageous for modeling composites because they predict overall composite response that does not follow macroscopic classical plasticity principles. Yielding under purely hydrostatic applied stress and a strain path-dependent, post-yield, mean stress-volumetric strain relation were shown in Fig. 4. Plastic compressibility, nonconvexity of regions of the effective yield surface, and absence of normality to it also occur. These failures of classical principles greatly complicate directly modeling the macroscopic response of composite materials. However, these principles remain applicable for many of the constituent materials and are

used in the MoC model. The three fiber aspect ratio examples of Fig. 8b and the anisotropy effects of Fig. 9 partially reveal the range of responses that the constitutive models and the homogenization technique can generate. Moreover, because the homogenization technique explicitly treats the mechanical response on the microstructural length scale and permits use of the well-understood, single phase constitutive models, the specific combination of material and microstructural contributions to any complex overall response of the composite can be identified. This is a great advantage of the MoC homogenization technique combined with accurate, physically-based constitutive models.

The present work demonstrates that the MoC homogenization technique is of practical use as a material model in continuum mechanics computer programs for simulating structural response of composites. The first order version of the model cannot represent any transient wave phenomena and all dynamic response associated with the microstructure of the RVE is absent from simulations. The leading order elastic nonlinearity has been incorporated into the model in a consistent manner using second- and third-order elastic constants. The model was implemented in one-dimensional and three-dimensional continuum mechanics computer programs. Elastic nonlinearity was shown to make significant contributions to structural response in high-rate loadings relevant to crash response, armor, and munitions applications. A practical but accurate approximation was presented for treating elastic nonlinearity in an isotropic matrix reinforced by strong, anisotropic, brittle fibers. A similar approximation for anisotropic matrix materials is desirable to mitigate the common absence of complete sets of third-order elastic constants.

An approach for calibrating the micromechanical model was also presented. Linear elastic moduli of an isotropic matrix were determined from acoustic wave speed and density measurements. Elastic moduli of the fiber were inferred from measured acoustic wave speeds in the composite. Lacking a sufficient variety of acoustic wave speeds, the measured speeds were augmented with data for similar materials. Nonlinear contributions to the matrix bulk modulus were determined from an assumed linear shock velocity/particle velocity relation. The coefficients of this relation can be obtained from as

few as two uniaxial strain impact experiments. Due to a lack of sufficient shock-wave data for the present epoxy, the coefficients were estimated from shock-wave data for similar materials. This information and the thermal expansivity or Grüneisen parameter are used in a standard EOS to represent the nonlinear elasticity effects. In the absence of damage, specification of the model is completed with a description of the matrix material inelastic response. Here, a viscoplasticity model was calibrated with uniaxial stress and Hopkinson bar measurements that spanned strain rates from 10^{-4} s^{-1} to 3000 s^{-1} .

Future work will focus on two immediate goals. The first is developing an approximate treatment of elastic nonlinearity in anisotropic constituent materials, as already noted. The second is to extend the present homogenization technique to treat laminates composed of fiber reinforced matrix layers. This extension will include a delamination model, as well as a homogenization of constituents within each layer that is consistent with homogenization of layers within the laminate. The resulting homogenization procedure will be useful for reducing the size of large scale numerical simulations by allowing each computational cell to contain many layering sequences, rather than only one layer.

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APPENDIX A. Relations Among Stress Moments and Stress Expansion Coefficients

The subcell-averaged stress moments are defined as⁶

$$S_{ij(pq)}^{\alpha\gamma} \equiv \frac{1}{d_\alpha h_\gamma} \int_{-d_\alpha/2}^{d_\alpha/2} dy_2^\alpha (y_2^\alpha)^p \int_{-h_\gamma/2}^{h_\gamma/2} dy_3^\gamma (y_3^\gamma)^q \sigma_{ij}^{\alpha\gamma} . \quad (A1)$$

The stress expansion for a continuous-fiber composite is⁶

$$\sigma_{ij}^{\alpha\gamma} = \sum_{m,n=0}^{N-1} [(1+2m)(1+2n)]^{1/2} \tau_{ij(mn)}^{\alpha\gamma} P_m(2y_2^\alpha/d_\alpha) P_n(2y_3^\gamma/h_\gamma) , \quad m+n < N . \quad (A2)$$

The restriction on the expansion indices ensures consistency with the strain expansion that follows from Eqs. (1) and (3). Aboudi has given the general relation between stress expansion coefficients $\tau_{ij(mn)}^{\alpha\gamma}$ and the stress moments.⁶ The relations appropriate for the $N = 3$ stress expansion are

$$S_{ij}^{\alpha\gamma} \equiv S_{ij(00)}^{\alpha\gamma} = \tau_{ij(00)}^{\alpha\gamma} , \quad \text{note abbreviation here;} \quad (A3)$$

$$S_{ij(10)}^{\alpha\gamma} = \frac{1}{2\sqrt{3}} d_\alpha \tau_{ij(10)}^{\alpha\gamma} ; \quad S_{ij(01)}^{\alpha\gamma} = \frac{1}{2\sqrt{3}} h_\gamma \tau_{ij(01)}^{\alpha\gamma} ; \quad S_{ij(11)}^{\alpha\gamma} = \frac{1}{12} d_\alpha h_\gamma \tau_{ij(11)}^{\alpha\gamma} ;$$

$$S_{ij(20)}^{\alpha\gamma} = \frac{1}{12} d_\alpha^2 \left[\tau_{ij(00)}^{\alpha\gamma} + \frac{2}{\sqrt{5}} \tau_{ij(20)}^{\alpha\gamma} \right] ; \quad S_{ij(02)}^{\alpha\gamma} = \frac{1}{12} h_\gamma^2 \left[\tau_{ij(00)}^{\alpha\gamma} + \frac{2}{\sqrt{5}} \tau_{ij(02)}^{\alpha\gamma} \right] ;$$

$$S_{ij(21)}^{\alpha\gamma} = d_\alpha^2 h_\gamma \left[\frac{\sqrt{3}}{72} \tau_{ij(01)}^{\alpha\gamma} + \frac{\sqrt{15}}{80} \tau_{ij(21)}^{\alpha\gamma} \right] ; \quad S_{ij(12)}^{\alpha\gamma} = d_\alpha h_\gamma^2 \left[\frac{\sqrt{3}}{72} \tau_{ij(10)}^{\alpha\gamma} + \frac{\sqrt{15}}{80} \tau_{ij(12)}^{\alpha\gamma} \right] ;$$

$$S_{ij(22)}^{\alpha\gamma} = \frac{1}{144} d_\alpha^2 h_\gamma^2 \left[\tau_{ij(00)}^{\alpha\gamma} + \frac{2}{d_\alpha \sqrt{5}} \tau_{ij(20)}^{\alpha\gamma} + \frac{2}{h_\gamma \sqrt{5}} \tau_{ij(02)}^{\alpha\gamma} \right] .$$

Hence, the zero- and first-order stress moments are proportional to the corresponding stress coefficients.

APPENDIX B. Stress Moment Equations of Motion for $N = 2$

As an illustration of stress moment equations of motion, Eq. (30) is expanded for the case $N = 2$. Relations among the integrals appearing in these stress-moment equations are obtained by expressing each in terms of the stress coefficients of Eq. (A2) in Appendix A. The boundary values of the stress are

$$\begin{aligned} \frac{1}{2} \left(\left[\sigma_{2j}^{\alpha\gamma} \right]_{y_2^\alpha = d_\alpha/2} + (-1)^{p+1} \left[\sigma_{2j}^{\alpha\gamma} \right]_{y_2^\alpha = -d_\alpha/2} \right) &= \sqrt{3} \tau_{2j(10)}^{\alpha\gamma}, \quad p \text{ even} \quad (B1) \\ &= \tau_{2j(00)}^{\alpha\gamma} + \frac{2\sqrt{3}}{h_\gamma} y_3^\gamma \tau_{2j(01)}^{\alpha\gamma}, \quad p \text{ odd} \end{aligned}$$

$$\begin{aligned} \frac{1}{2} \left(\left[\sigma_{3j}^{\alpha\gamma} \right]_{y_3^\gamma = h_\gamma/2} + (-1)^{q+1} \left[\sigma_{3j}^{\alpha\gamma} \right]_{y_3^\gamma = -h_\gamma/2} \right) &= \sqrt{3} \tau_{3j(01)}^{\alpha\gamma}, \quad q \text{ even} \quad (B2) \\ &= \tau_{3j(00)}^{\alpha\gamma} + \frac{2\sqrt{3}}{d_\alpha} \tau_{3j(10)}^{\alpha\gamma} y_2^\alpha, \quad q \text{ odd}. \end{aligned}$$

Substituting these results into Eqs. (31) and (32), integrating, and comparing with Eq. (A3), Appendix A, leads to the following relations:

$$\begin{aligned} I_{2j(00)}^{\alpha\gamma} &= \frac{12}{d_\alpha^2} S_{2j(10)}^{\alpha\gamma}, & J_{3j(00)}^{\alpha\gamma} &= \frac{12}{h_\gamma^2} S_{3j(01)}^{\alpha\gamma}, & (B3) \\ I_{2j(10)}^{\alpha\gamma} &= S_{2j(00)}^{\alpha\gamma}, & J_{3j(10)}^{\alpha\gamma} &= \frac{12}{h_\gamma^2} S_{3j(11)}^{\alpha\gamma}, \\ I_{2j(01)}^{\alpha\gamma} &= \frac{12}{d_\alpha^2} S_{2j(11)}^{\alpha\gamma}, & J_{3j(01)}^{\alpha\gamma} &= S_{3j(00)}^{\alpha\gamma}, \\ I_{2j(11)}^{\alpha\gamma} &= S_{2j(01)}^{\alpha\gamma}, & J_{3j(11)}^{\alpha\gamma} &= S_{3j(10)}^{\alpha\gamma}, \end{aligned}$$

$$I_{2j(20)}^{\alpha\gamma} = 3S_{2j(10)}^{\alpha\gamma}, \quad J_{3j(20)}^{\alpha\gamma} = \left(\frac{d_\alpha}{h_\gamma}\right)^2 S_{3j(01)}^{\alpha\gamma},$$

$$I_{2j(02)}^{\alpha\gamma} = \left(\frac{h_\gamma}{d_\alpha}\right)^2 S_{2j(10)}^{\alpha\gamma}, \quad J_{3j(02)}^{\alpha\gamma} = 3S_{3j(01)}^{\alpha\gamma},$$

$$\begin{aligned} I_{2j(21)}^{\alpha\gamma} &= 3S_{2j(11)}^{\alpha\gamma}, & J_{3j(21)}^{\alpha\gamma} &= \frac{d_\alpha^2}{12} S_{3j(00)}^{\alpha\gamma}, \\ I_{2j(21)}^{\alpha\gamma} &= \frac{h_\gamma^2}{12} S_{2j(00)}^{\alpha\gamma}, & J_{3j(22)}^{\alpha\gamma} &= 3S_{3j(11)}^{\alpha\gamma}, \\ I_{2j(22)}^{\alpha\gamma} &= \frac{h_\gamma^2}{12} S_{2j(10)}^{\alpha\gamma}, & J_{3j(22)}^{\alpha\gamma} &= \frac{d_\alpha^2}{12} S_{3j(01)}^{\alpha\gamma}. \end{aligned}$$

Using Eq. (1) with $N = 2$, (B3), and (A3), the stress-moment equations, Eq. (30), becomes

$$\begin{matrix} p & q \\ 0 & 0 \end{matrix} \quad \partial_1 \tau_{1j(00)}^{\alpha\gamma} + \frac{2\sqrt{3}}{d_\alpha} \tau_{2j(10)}^{\alpha\gamma} + \frac{2\sqrt{3}}{h_\gamma} \tau_{3j(01)}^{\alpha\gamma} = \rho_{\alpha\gamma} \ddot{U}_{j(00)}^{\alpha\gamma}, \quad (B4a)$$

$$\begin{matrix} 1 & 0 \end{matrix} \quad \partial_1 \tau_{1j(10)}^{\alpha\gamma} = \frac{\rho_{\alpha\gamma}}{\sqrt{3}} \ddot{U}_{j(10)}^{\alpha\gamma}, \quad (B4b)$$

$$\begin{matrix} 0 & 1 \end{matrix} \quad \partial_1 \tau_{1j(01)}^{\alpha\gamma} = \frac{\rho_{\alpha\gamma}}{\sqrt{3}} \ddot{U}_{j(01)}^{\alpha\gamma}, \quad (B4c)$$

$$\begin{matrix} 1 & 1 \end{matrix} \quad 0 = \frac{\rho_{\alpha\gamma}}{3} \ddot{U}_{j(11)}^{\alpha\gamma}, \quad (B4d)$$

$$\begin{matrix} 2 & 0 \end{matrix} \quad \partial_1 \tau_{1j(00)}^{\alpha\gamma} + \frac{2\sqrt{3}}{d_\alpha} \tau_{2j(10)}^{\alpha\gamma} + \frac{2\sqrt{3}}{h_\gamma} \tau_{3j(01)}^{\alpha\gamma} = \rho_{\alpha\gamma} \left(\ddot{U}_{j(00)}^{\alpha\gamma} + \frac{2}{5} \ddot{U}_{j(20)}^{\alpha\gamma} \right), \quad (B4e)$$

$$\begin{matrix} 0 & 2 \end{matrix} \quad \partial_1 \tau_{1j(00)}^{\alpha\gamma} + \frac{2\sqrt{3}}{d_\alpha} \tau_{2j(10)}^{\alpha\gamma} + \frac{2\sqrt{3}}{h_\gamma} \tau_{3j(01)}^{\alpha\gamma} = \rho_{\alpha\gamma} \left(\ddot{U}_{j(00)}^{\alpha\gamma} + \frac{2}{5} \ddot{U}_{j(02)}^{\alpha\gamma} \right), \quad (B4f)$$

$$2 \ 1 \quad \partial_1 \tau_{1j(01)}^{\alpha\gamma} = \frac{\rho_{\alpha\gamma}}{\sqrt{3}} \dot{U}_{j(01)}^{\alpha\gamma}, \quad (\text{B4g})$$

$$1 \ 2 \quad \partial_1 \tau_{1j(10)}^{\alpha\gamma} = \frac{\rho_{\alpha\gamma}}{\sqrt{3}} \dot{U}_{j(10)}^{\alpha\gamma}, \quad (\text{B4h})$$

$$2 \ 2 \quad \partial_1 \tau_{1j(00)}^{\alpha\gamma} - \frac{2\sqrt{3}}{d_\alpha} \tau_{2j(10)}^{\alpha\gamma} - \frac{2\sqrt{3}}{h_\gamma} \tau_{3j(01)}^{\alpha\gamma} = \rho_{\alpha\gamma} \left(\dot{U}_{j(00)}^{\alpha\gamma} + \frac{2}{5} \dot{U}_{j(20)}^{\alpha\gamma} + \frac{2}{5} \dot{U}_{j(02)}^{\alpha\gamma} \right). (\text{B4i})$$

This hierarchy of stress-moment equations continues, without duplicating the six relations, Eqs. (B4a) through (B4f). These six vector equations for each subcell involve all six of the displacement expansion vector coefficients of Eq. (1). [Equations (B4a), (B4e), and (B4f) immediately yield $\dot{U}_{j(00)}^{\alpha\gamma} = \dot{U}_{j(20)}^{\alpha\gamma} = 0$.] With initial and boundary conditions, and subcell traction and displacement conditions, it should be possible to solve these six equations for the time histories of the 36 displacement and stress coefficients per subcell. Presuming this set of relations is solvable, it is reasonable to truncate the hierarchy of stress-moment equations by omitting all equations for which $p + q > N$. No other criterion for closing the series of equations is evident.

For $N = 2$, traction continuity provides six independent vector relations for the stress coefficients. For this case, Eqs. (33a, b) reduce to

$$I_{2j(pq)}^{1\gamma} = \left(-\frac{d_1}{d_2} \right)^{p-1} I_{2j(pq)}^{2\gamma} - \frac{2D}{h_\gamma} \left(\frac{d_1}{2} \right)^{p-1} \frac{\partial}{\partial x_2} \left(\tau_{2i(0,0)}^{2\gamma} \right) \int_{-h_\gamma/2}^{h_\gamma/2} dy_3^\gamma (y_3^\gamma)^q \quad (\text{B5a})$$

and

$$J_{3j(pq)}^{\alpha 1} = \left(-\frac{h_1}{h_2} \right)^{q-1} J_{3j(pq)}^{\alpha 2} - \frac{2H}{d_\alpha} \left(\frac{h_1}{2} \right)^{q-1} \frac{\partial}{\partial x_3} \left(\tau_{3i(m,n)}^{\alpha 2} \right) \int_{-d_\alpha/2}^{d_\alpha/2} dy_2^\alpha (y_2^\alpha)^p. \quad (\text{B5b})$$

Substituting into these expressions from Eqs. (B3) and (A3) for each (p, q) yields,

p q	Eq. (31a)	Eq. (31b)
0 0	$\tau_{2j(10)}^{1\gamma} = -\tau_{2j(10)}^{2\gamma} + \frac{2D}{\sqrt{3}} \frac{\partial \tau_{2j(0,0)}^{2\gamma}}{\partial x_2},$	$\tau_{3j(01)}^{\alpha 1} = -\tau_{3j(01)}^{\alpha 2} + \frac{2H}{\sqrt{3}} \frac{\partial \tau_{3j(0,0)}^{\alpha 2}}{\partial x_3},$ (B6a,b)
1 0	$\tau_{2j(00)}^{1\gamma} = \tau_{2j(00)}^{2\gamma} - 2D \frac{\partial \tau_{2j(0,0)}^{2\gamma}}{\partial x_2},$	$0 = 0,$ (B7a,b)
0 1	$0 = 0,$	$\tau_{3j(00)}^{\alpha 1} = \tau_{3j(00)}^{\alpha 2} - 2H \frac{\partial \tau_{3j(0,0)}^{\alpha 2}}{\partial x_3},$ (B8a,b)
1 1	$\tau_{2j(01)}^{1\gamma} = \tau_{2j(01)}^{2\gamma},$	$\tau_{3j(10)}^{\alpha 1} = \tau_{3j(10)}^{\alpha 2}.$ (B9a,b)

The relations for (p, q) = (2, 0) and (0, 2) are redundant. For N = 2, displacement continuity Eqs. (20), (21), (22), and (23), respectively, are

$$-\partial_2 \underline{U}_{(00)}^{1\gamma} - \frac{D}{2} \partial_2^2 \underline{U}_{(00)}^{1\gamma} + \partial_2 \underline{U}_{(10)}^{1\gamma} = -\partial_2 \underline{U}_{(00)}^{2\gamma} + \frac{D}{2} \partial_2^2 \underline{U}_{(00)}^{2\gamma} - \partial_2 \underline{U}_{(10)}^{2\gamma}; \quad (B10)$$

$$\frac{2}{D} (\underline{U}_{(10)}^{1\gamma} + \underline{U}_{(10)}^{2\gamma}) = \partial_2 \underline{U}_{(00)}^{1\gamma} + \frac{D}{2} \partial_2^2 \underline{U}_{(00)}^{1\gamma} - \partial_2 \underline{U}_{(10)}^{1\gamma}; \quad (B11)$$

$$-\partial_3 \underline{U}_{(00)}^{\alpha 1} - \frac{H}{2} \partial_3^2 \underline{U}_{(00)}^{\alpha 1} + \partial_3 \underline{U}_{(01)}^{\alpha 1} = -\partial_3 \underline{U}_{(00)}^{\alpha 2} + \frac{H}{2} \partial_3^2 \underline{U}_{(00)}^{\alpha 2} - \partial_3 \underline{U}_{(01)}^{\alpha 2}; \quad (B12)$$

$$\frac{2}{H} (\underline{U}_{(01)}^{\alpha 1} + \underline{U}_{(01)}^{\alpha 2}) = \partial_3 \underline{U}_{(00)}^{\alpha 1} + \frac{H}{2} \partial_3^2 \underline{U}_{(00)}^{\alpha 1} - \partial_3 \underline{U}_{(01)}^{\alpha 1}. \quad (B13)$$

The relations for the first-order model (N = 1) are obtained from Eqs. (B4) and (B6) through (B13) by omitting stress coefficients of order m + n > 0, displacement coefficients of order m + n > 1, and second derivatives. Also, the gradients of $\tau_{ij(00)}^{\alpha\gamma}$ are omitted from

Eqs. (B6) through (B9). Doing this it is seen that Eq. (B4a) is the only nontrivial stress-moment equation,

$$\partial_1 \tau_{1j(00)}^{\alpha\gamma} = \rho_{\alpha\gamma} \ddot{U}_{j(00)}^{\alpha\gamma} \quad . \quad (B14)$$

Equations (B7a) and (B8b) are the only nontrivial traction continuity equations, and Eqs. (B10) through (B13) reduce to Eqs. (39a,b) and (40a,b), respectively. Upon asserting Eq. (41), the coefficients $\partial_i \underline{U}_{(00)}^{\alpha\gamma}$ are identified as the (macroscopic) displacement gradients in the homogenized continuum. Hence, $\underline{U}_{(00)}^{\alpha\gamma}$ correspond to macroscopic displacements to within a constant. Because the variation with respect to the macroscopic coordinate x_1 is the same for each subcell, the quantity $\partial_1 \tau_{1j(00)}^{\alpha\gamma}$, too, is a macroscopic quantity. Equation (B14) is thus seen to relate macroscopic quantities. Consequently, dynamic effects do not contribute to the microstructural response unless a second- or higher-order treatment is performed.

For application as the material model in a numerical continuum mechanics (CM) calculation, the static solution of the MoC model relations to specified macroscopic velocity gradient values can be determined readily. In a finite element method (FEM) calculation, for example, the velocity gradients are known for each computational cell at each computational time step. A consequence of using the static solution to the MoC relations is that no wave effects due to microstructure are determined, even when a higher-order description is used. The dynamic response of a composite can be determined only for wavelengths comparable to the RVE size, or larger. In the second-order description, the macroscopic derivatives of the displacement gradients, $\partial_i^2 \underline{U}_{(00)}^{\alpha\gamma}$, and those of the first-order displacement coefficients and zero-order stress coefficients, which occur in Eqs. (B6) through (B13), must be estimated from the values of displacement gradient, and displacement and stress coefficients in neighboring computational cells. If, instead, these quantities are taken to be zero, the static solution for the first-order description is recovered.

In the first-order description, the static solution leaves $\partial_1 \tau_{1j(00)}^{\alpha\gamma} = 0$, from Eq. (B14). Because this macroscopic quantity is determined by the CM simulation, this equation does not affect the microstructural model solution. Hence, for the static solution, the coefficients are completely determined from the displacement continuity and traction conditions, as described in the main text. In the second-order description, the static microstructural model solution must additionally satisfy Eqs. (B4a) and (B4e). These stress-moment equations are satisfied provided

$$\partial_1 \tau_{1j(00)}^{\alpha\gamma} + \frac{2\sqrt{3}}{d_\alpha} \tau_{2j(10)}^{\alpha\gamma} + \frac{2\sqrt{3}}{h_\gamma} \tau_{3j(01)}^{\alpha\gamma} = 0. \quad (\text{B15})$$

The static solution exists if the coefficients are determined from the 72 scalar subcell equations (B6) through (B13) and (B15), assuming Eq. (41) applies. The 72 displacement coefficients cannot all be determined because stress tensor symmetry makes three scalar equations from Eqs. (B6) through (B9) dependent. From Eqs. (B6a) and (B9b), only three of four equations of the form

$$\tau_{23(10)}^{\alpha\gamma} = -\tau_{23(10)}^{\alpha\gamma} \quad (\text{B16})$$

are independent. The situation is similar for Eqs. (B6b) and (B9a), and for Eqs. (B7) and (B8). Hence, at best 66 of the displacement coefficients can be determined along with three linear combinations of two coefficients each.

APPENDIX C. Cauchy Stress to Second Order in Small Strain for Orthorhombic Symmetry

Orthorhombic symmetry corresponds to 9 unique SOECs and 20 unique TOECs with only elastic constants related by interchange of Voigt indices being equal. In Voigt notation (see section VI), these elastic constants are^{14,17}

$$\text{SOEC: } C_{11}, C_{22}, C_{33}, C_{23}, C_{13}, C_{12}, C_{44}, C_{55}, C_{66}. \quad (\text{C1})$$

$$\text{TOEC: } C_{111}, C_{112}, C_{113}, C_{122}, C_{123}, C_{133}, C_{144}, C_{155}, C_{166}, \\ C_{222}, C_{223}, C_{233}, C_{244}, C_{255}, C_{266}, C_{333}, C_{334}, C_{335}, C_{366}, C_{456}. \quad (\text{C2})$$

Performing the summations implied in Eq. (53) for this material symmetry yields

$$\begin{aligned} \sigma_1 &= C_{11} e_1 + C_{12} e_2 + C_{13} e_3 \quad (\text{C3}) \\ &+ \frac{1}{2} e_1^2 (C_{111} + 3C_{11}) + \frac{1}{2} e_2^2 (C_{122} - C_{12}) + \frac{1}{2} e_3^2 (C_{133} - C_{13}) \\ &+ e_1 e_2 (C_{112} - C_{11} + C_{12}) + e_2 e_3 (C_{123} - C_{12} - C_{13}) + e_3 e_1 (C_{113} - C_{11} + C_{13}) \\ &+ \frac{1}{8} e_4^2 (4C_{144} + C_{12} + C_{13}) \\ &+ \frac{1}{8} e_5^2 (4C_{155} + C_{11} + C_{13} + 8C_{55}) + \frac{1}{8} e_6^2 (4C_{166} + C_{11} + C_{12} + 8C_{66}); \end{aligned}$$

$$\begin{aligned} \sigma_2 &= C_{12} e_1 + C_{22} e_2 + C_{23} e_3 \quad (\text{C4}) \\ &+ \frac{1}{2} e_1^2 (C_{112} - C_{12}) + \frac{1}{2} e_2^2 (C_{222} + 3C_{22}) + \frac{1}{2} e_3^2 (C_{233} - C_{23}) \\ &+ e_1 e_2 (C_{122} - C_{22} + C_{12}) + e_2 e_3 (C_{223} - C_{22} + C_{23}) + e_3 e_1 (C_{123} - C_{12} - C_{23}) \\ &+ \frac{1}{8} e_4^2 (4C_{244} + C_{22} + C_{23} + 8C_{44}) \\ &+ \frac{1}{8} e_5^2 (4C_{255} + C_{12} + C_{23}) + \frac{1}{8} e_6^2 (4C_{266} + C_{12} + C_{22} + 8C_{66}); \end{aligned}$$

$$\begin{aligned} \sigma_3 &= C_{13} e_1 + C_{23} e_2 + C_{33} e_3 \quad (\text{C5}) \\ &+ \frac{1}{2} e_1^2 (C_{113} - C_{13}) + \frac{1}{2} e_2^2 (C_{223} - C_{23}) + \frac{1}{2} e_3^2 (C_{333} + 3C_{33}) \\ &+ e_1 e_2 (C_{123} - C_{13} + C_{23}) + e_2 e_3 (C_{233} - C_{33} + C_{23}) + e_3 e_1 (C_{133} - C_{33} + C_{13}) \\ &+ \frac{1}{8} e_4^2 (4C_{344} + C_{23} + C_{33} + 8C_{44}) \end{aligned}$$

$$+ \frac{1}{8} e_5^2 (4C_{355} + C_{13} + C_{33} + 8C_{55}) + \frac{1}{8} e_6^2 (4C_{366} + C_{13} + C_{23});$$

$$\begin{aligned} \sigma_4 = & C_{44} e_4 + \frac{1}{2} e_5 e_6 \left(\frac{1}{2} C_{44} + C_{55} + C_{66} + 2C_{456} \right) \\ & + \frac{1}{2} e_4 [e_1 (2C_{144} + C_{12} + C_{13} - 2C_{44}) + e_2 (2C_{244} + C_{22} + C_{23} + C_{44}) \\ & + e_3 (2C_{344} + C_{23} + C_{33} + C_{44})]; \end{aligned} \quad (C6)$$

$$\begin{aligned} \sigma_5 = & C_{55} e_5 + \frac{1}{2} e_6 e_4 \left(C_{44} + \frac{1}{2} C_{55} + C_{66} + 2C_{456} \right) \\ & + \frac{1}{2} e_5 [e_1 (2C_{155} + C_{11} + C_{13} + C_{55}) + e_2 (2C_{255} + C_{12} + C_{23} - 2C_{55}) \\ & + e_3 (2C_{355} + C_{13} + C_{33} + C_{55})]; \end{aligned} \quad (C7)$$

$$\begin{aligned} \sigma_6 = & C_{66} e_6 + \frac{1}{2} e_4 e_5 \left(C_{44} + C_{55} + \frac{1}{2} C_{66} + 2C_{456} \right) \\ & + \frac{1}{2} e_6 [e_1 (2C_{166} + C_{11} + C_{12} + C_{66}) + e_2 (2C_{266} + C_{12} + C_{22} + C_{66}) \\ & + e_3 (2C_{366} + C_{12} + C_{13} - 2C_{66})]. \end{aligned} \quad (C8)$$

Using these nonlinear stress/strain relations and Eq. (36), for a continuous fiber-reinforced matrix, the subcell stress expressions in first order MoC are given by the following:

$$\begin{aligned} S_1^{\alpha\gamma} = & S_{1(o)}^{\alpha\gamma} + a_1^{\alpha\gamma} (\bar{\epsilon}_1 - L_1^{\alpha\gamma}) (\phi_2^{\alpha\gamma} - L_2^{\alpha\gamma}) + b_1^{\alpha\gamma} (\phi_2^{\alpha\gamma} - L_2^{\alpha\gamma}) (\psi_3^{\alpha\gamma} - L_3^{\alpha\gamma}) \\ & + e_1^{\alpha\gamma} (\psi_3^{\alpha\gamma} - L_3^{\alpha\gamma}) (\bar{\epsilon}_1 - L_1^{\alpha\gamma}) + f_1^{\alpha\gamma} (\bar{\epsilon}_1 - L_1^{\alpha\gamma})^2 \\ & + k_1^{\alpha\gamma} (\phi_2^{\alpha\gamma} - L_2^{\alpha\gamma})^2 + m_1^{\alpha\gamma} (\psi_3^{\alpha\gamma} - L_3^{\alpha\gamma})^2 \\ & + \frac{1}{4} g_1^{\alpha\gamma} [\zeta^{\alpha\gamma} - L_4^{\alpha\gamma}]^2 + \frac{1}{4} i_1^{\alpha\gamma} [w_{3,1} + \psi_1^{\alpha\gamma} - L_5^{\alpha\gamma}]^2 \\ & + \frac{1}{4} j_1^{\alpha\gamma} [w_{2,1} + \phi_1^{\alpha\gamma} - L_6^{\alpha\gamma}]^2; \end{aligned} \quad (C9)$$

$$\begin{aligned} S_2^{\alpha\gamma} = & S_{2(o)}^{\alpha\gamma} + a_2^{\alpha\gamma} (\bar{\epsilon}_1 - L_1^{\alpha\gamma}) (\phi_2^{\alpha\gamma} - L_2^{\alpha\gamma}) + b_2^{\alpha\gamma} (\phi_2^{\alpha\gamma} - L_2^{\alpha\gamma}) (\psi_3^{\alpha\gamma} - L_3^{\alpha\gamma}) \\ & + e_2^{\alpha\gamma} (\psi_3^{\alpha\gamma} - L_3^{\alpha\gamma}) (\bar{\epsilon}_1 - L_1^{\alpha\gamma}) + k_2^{\alpha\gamma} (\bar{\epsilon}_1 - L_1^{\alpha\gamma})^2 \\ & + f_2^{\alpha\gamma} (\phi_2^{\alpha\gamma} - L_2^{\alpha\gamma})^2 + m_2^{\alpha\gamma} (\psi_3^{\alpha\gamma} - L_3^{\alpha\gamma})^2 \end{aligned} \quad (C10)$$

$$+ \frac{1}{4} g_2^{\alpha\gamma} [\zeta^{\alpha\gamma} - L_4^{\alpha\gamma}]^2 + \frac{1}{4} i_2^{\alpha\gamma} [w_{3,1} + \psi_1^{\alpha\gamma} - L_5^{\alpha\gamma}]^2 \\ + \frac{1}{4} j_2^{\alpha\gamma} [w_{2,1} + \phi_1^{\alpha\gamma} - L_6^{\alpha\gamma}]^2 ;$$

$$S_3^{\alpha\gamma} = S_{3(o)}^{\alpha\gamma} + a_3^{\alpha\gamma} (\bar{\epsilon}_1 - L_1^{\alpha\gamma}) (\phi_2^{\alpha\gamma} - L_2^{\alpha\gamma}) + b_3^{\alpha\gamma} (\phi_2^{\alpha\gamma} - L_2^{\alpha\gamma}) (\psi_3^{\alpha\gamma} - L_3^{\alpha\gamma}) \\ + e_3^{\alpha\gamma} (\psi_3^{\alpha\gamma} - L_3^{\alpha\gamma}) (\bar{\epsilon}_1 - L_1^{\alpha\gamma}) + k_3^{\alpha\gamma} (\bar{\epsilon}_1 - L_1^{\alpha\gamma})^2 \\ + m_3^{\alpha\gamma} (\phi_2^{\alpha\gamma} - L_2^{\alpha\gamma})^2 + f_3^{\alpha\gamma} (\psi_3^{\alpha\gamma} - L_3^{\alpha\gamma})^2 \\ + \frac{1}{4} g_3^{\alpha\gamma} [\zeta^{\alpha\gamma} - L_4^{\alpha\gamma}]^2 + \frac{1}{4} i_3^{\alpha\gamma} [w_{3,1} + \psi_1^{\alpha\gamma} - L_5^{\alpha\gamma}]^2 \\ + \frac{1}{4} j_3^{\alpha\gamma} [w_{2,1} + \phi_1^{\alpha\gamma} - L_6^{\alpha\gamma}]^2 ; \quad (C11)$$

$$S_4^{\alpha\gamma} = S_{4(o)}^{\alpha\gamma} + f_4^{\alpha\gamma} (w_{3,1} + \psi_1^{\alpha\gamma} - L_5^{\alpha\gamma}) (w_{2,1} + \phi_1^{\alpha\gamma} - L_6^{\alpha\gamma}) + \\ \frac{1}{2} (\zeta^{\alpha\gamma} - L_4^{\alpha\gamma}) [a_4^{\alpha\gamma} (\bar{\epsilon}_1 - L_1^{\alpha\gamma}) + b_4^{\alpha\gamma} (\phi_2^{\alpha\gamma} - L_2^{\alpha\gamma}) + e_4^{\alpha\gamma} (\psi_3^{\alpha\gamma} - L_3^{\alpha\gamma})] ; \quad (C12)$$

$$S_5^{\alpha\gamma} = S_{5(o)}^{\alpha\gamma} + f_5^{\alpha\gamma} (w_{2,1} + \phi_1^{\alpha\gamma} - L_6^{\alpha\gamma}) (\zeta^{\alpha\gamma} - L_4^{\alpha\gamma}) + \frac{1}{2} (w_{3,1} + \psi_1^{\alpha\gamma} - L_5^{\alpha\gamma}) \times \\ [a_5^{\alpha\gamma} (\bar{\epsilon}_1 - L_1^{\alpha\gamma}) + b_5^{\alpha\gamma} (\phi_2^{\alpha\gamma} - L_2^{\alpha\gamma}) + e_5^{\alpha\gamma} (\psi_3^{\alpha\gamma} - L_3^{\alpha\gamma})] ; \quad (C13)$$

$$S_6^{\alpha\gamma} = S_{6(o)}^{\alpha\gamma} + f_6^{\alpha\gamma} (w_{3,1} + \psi_1^{\alpha\gamma} - L_5^{\alpha\gamma}) (\zeta^{\alpha\gamma} - L_4^{\alpha\gamma}) + \frac{1}{2} (w_{2,1} + \phi_1^{\alpha\gamma} - L_6^{\alpha\gamma}) \\ [a_6^{\alpha\gamma} (\bar{\epsilon}_1 - L_1^{\alpha\gamma}) + b_6^{\alpha\gamma} (\phi_2^{\alpha\gamma} - L_2^{\alpha\gamma}) + e_6^{\alpha\gamma} (\psi_3^{\alpha\gamma} - L_3^{\alpha\gamma})] ; \quad (C14)$$

where

$$S_{1(o)}^{\alpha\gamma} = (\bar{\epsilon}_1 - L_1^{\alpha\gamma}) C_{11}^{\alpha\gamma} + (\phi_2^{\alpha\gamma} - L_2^{\alpha\gamma}) C_{12}^{\alpha\gamma} + (\psi_3^{\alpha\gamma} - L_3^{\alpha\gamma}) C_{13}^{\alpha\gamma} ; \quad (C15)$$

$$S_{2(o)}^{\alpha\gamma} = (\bar{\epsilon}_1 - L_1^{\alpha\gamma}) C_{12}^{\alpha\gamma} + (\phi_2^{\alpha\gamma} - L_2^{\alpha\gamma}) C_{22}^{\alpha\gamma} + (\psi_3^{\alpha\gamma} - L_3^{\alpha\gamma}) C_{23}^{\alpha\gamma} ; \quad (C16)$$

$$S_{3(o)}^{\alpha\gamma} = (\bar{\epsilon}_1 - L_1^{\alpha\gamma}) C_{13}^{\alpha\gamma} + (\phi_2^{\alpha\gamma} - L_2^{\alpha\gamma}) C_{23}^{\alpha\gamma} + (\psi_3^{\alpha\gamma} - L_3^{\alpha\gamma}) C_{33}^{\alpha\gamma} ; \quad (C17)$$

$$S_{4(o)}^{\alpha\gamma} = (\zeta^{\alpha\gamma} - L_4^{\alpha\gamma}) C_{44}^{\alpha\gamma} ; \quad (C18)$$

$$S_{5(o)}^{\alpha\gamma} = (w_{3,1} + \psi_1^{\alpha\gamma} - L_5^{\alpha\gamma}) C_{55}^{\alpha\gamma}; \quad (C19)$$

$$S_{6(o)}^{\alpha\gamma} = (w_{2,1} + \phi_1^{\alpha\gamma} - L_6^{\alpha\gamma}) C_{66}^{\alpha\gamma}. \quad (C20)$$

The elastic constant combinations are defined as follows. The subcell indices are omitted, but the "fiber" subcell $(\alpha\gamma) = (11)$ always needs be distinguished from the matrix subcells. In the absence of damage the other three subcells share the same constant values.

$$a_1 = C_{112} - C_{11} + C_{12} \quad (C21)$$

$$b_1 = C_{123} - C_{12} - C_{13}$$

$$e_1 = C_{113} - C_{11} + C_{13}$$

$$f_1 = \frac{1}{2}(C_{111} + 3C_{11})$$

$$g_1 = \frac{1}{2}(4C_{144} + C_{12} + C_{13})$$

$$i_1 = \frac{1}{2}(4C_{155} + C_{11} + C_{13} + 8C_{55})$$

$$j_1 = \frac{1}{2}(4C_{166} + C_{11} + C_{12} + 8C_{66})$$

$$k_1 = \frac{1}{2}(C_{122} - C_{12})$$

$$m_1 = \frac{1}{2}(C_{133} - C_{13})$$

$$a_2 = C_{122} + C_{12} - C_{22} \quad (C22)$$

$$b_2 = C_{223} + C_{23} - C_{22}$$

$$e_2 = C_{123} - C_{12} - C_{23}$$

$$f_2 = \frac{1}{2}(C_{222} + 3C_{22})$$

$$g_2 = \frac{1}{2}(4C_{244} + C_{22} + C_{23} + 8C_{44})$$

$$i_2 = \frac{1}{2}(4C_{255} + C_{12} + C_{23})$$

$$j_2 = \frac{1}{2}(4C_{266} + C_{12} + C_{22} + 8C_{66})$$

$$k_2 = \frac{1}{2}(C_{112} - C_{12})$$

$$m_2 = \frac{1}{2}(C_{233} - C_{23})$$

$$a_3 = C_{123} - C_{13} - C_{23} \quad (C23)$$

$$b_3 = C_{223} + C_{23} - C_{33}$$

$$e_3 = C_{113} + C_{13} - C_{33}$$

$$f_3 = \frac{1}{2}(C_{333} + 3C_{33})$$

$$g_3 = \frac{1}{2}(4C_{344} + C_{23} + C_{33} + 8C_{44})$$

$$i_3 = \frac{1}{2}(4C_{355} + C_{13} + C_{33} + 8C_{55})$$

$$j_3 = \frac{1}{2}(4C_{366} + C_{13} + C_{23})$$

$$k_3 = \frac{1}{2}(C_{113} - C_{13})$$

$$m_3 = \frac{1}{2}(C_{223} - C_{23})$$

$$a_4 = 2C_{144} + C_{12} + C_{13} - 2C_{44} \quad (C24)$$

$$b_4 = 2C_{244} + C_{22} + C_{23} + C_{44}$$

$$e_4 = 2C_{344} + C_{23} + C_{33} + C_{44}$$

$$f_4 = \frac{1}{4}(4C_{456} + C_{44} + 2C_{55} + 2C_{66})$$

$$a_5 = 2C_{155} + C_{11} + C_{13} + C_{55} \quad (C25)$$

$$b_5 = 2C_{255} + C_{12} + C_{23} - 2C_{55}$$

$$e_5 = 2C_{355} + C_{13} + C_{33} + C_{55}$$

$$f_5 = \frac{1}{4}(4C_{456} + 2C_{44} + C_{55} + 2C_{66})$$

$$a_6 = 2C_{166} + C_{11} + C_{12} + C_{66} \quad (C26)$$

$$b_6 = 2C_{266} + C_{12} + C_{22} + C_{66}$$

$$e_6 = 2C_{366} + C_{13} + C_{23} - 2C_{66}$$

$$f_6 = \frac{1}{4}(4C_{456} + 2C_{44} + 2C_{55} + C_{66}) .$$

APPENDIX D. Description of FONE: One-Cell Calculation of First-Order MoC Homogenization

OVERVIEW: FONE computes the subcell and average macroscopic responses to uniform loading of a unidirectional continuous fiber-reinforced composite. The uniform loading constraint arises from treating only one computational element. Laminates with homogeneous layers can also be simulated by choosing the subcell dimensions so that $h_2 \ll h_1$. The program computes the mechanical response according to Aboudi's first-order MoC model with either linear elasticity, as he used, or nonlinear elasticity, as described in section VI. The constituent materials are assumed to have orthorhombic symmetry and the Bodner-Partom viscoplasticity model is used as the deviatoric stress/plastic strain relation. Tensor indices are abbreviated according to the conventional Voigt notation, which includes factors of 2 for the off-diagonal strains; e.g., $\epsilon_4 = 2\epsilon_{23}$. Currently, the load paths implemented in the program are uniaxial strain; axial (along fiber) shear strain; transverse shear strain; arbitrary normal strain; arbitrary normal stress. "Normal" components are relative to coordinates of the composite where the fiber lies along the x_1 -direction and the x_2 - and x_3 -directions parallel the corresponding y -directions within the RVE. (The pure shear and the simple shear loading paths have not been debugged. Arbitrary applied strain loading can be easily implemented by modifying the subroutine PATH to accept the full strain tensor in laboratory coordinates and the rotation matrix that relates it to the composite coordinates.)

The input comprises the microstructural dimensions, constituent material properties, and loading path specifications. FONE has menu-driven input, but once a user is familiar with the input information it is quicker to enter it on consecutive lines of a text file. Execute FONE with an input file using the UNIX redirecting of standard input; i.e.,

fone.x < in.file ,

where fone.x is the executable file, "<" is the UNIX redirecting operator, and in.file is the input information.

Four text files are output. Each has a two-part name with the second part being an 8-character "job" name, which is entered as the first line of input. Information written to unit 14 is stored in a file with "msg." prefixed onto the job name. This is the MeSsaGe file. It echoes the input information and reports the job status upon termination. It can serve as a record of the calculation. The three remaining output files contain data written as a space-delimited table suitable for input into a spreadsheet/graphics program.

The data written to unit 15 is stored in a file with "mss." prefixed onto the job name, which denotes Macroscopic Stress and Strain. It contains histories of the homogenized stress and strain component values. Time in ms is given in the first column, followed by the six components of stress in GPa, six components of total strain, and finally the six components of plastic strain.

The data written to unit 16 is stored in a file with "scv." prefixed onto the job name, which denotes SubCell Variables. It contains histories of the individual subcell stress and strain component values. Column one contains time in ms. This is followed by the six stress components, six total strain components, and six plastic strain components for subcell (11). The same information for subcells (21), (12), and (22), respectively, is given in the succeeding columns.

The data written to unit 17 is stored in a file with "rsd." prefixed onto the job name, which stands for ReSiDuals. It contains the residuals from the iterative solution for the microvariables. (If the residual and the "left-hand side" of the Taylor series are zero, a "5." appears in the table. If only the residual is zero, a "1." appears in the table.) The first column gives the time in ms. Succeeding columns give the residuals for 11 stress continuity expressions. No residuals for the macroscopic stress expressions are given, though these are used in applied stress loading.

The 11 subroutines are alphabetically ordered, except for DISER, which is the applied-stress version of RESID and appears last. Common blocks are referenced in the main program and subroutines by "include" statements. They are all contained in the file

"clues.comm," which needs to be in the directory with the main program and 11 subroutines when the "make" command is issued to compile the program.

MAIN: FORTRAN variable definitions are given in comments at the beginning of the listing. The constituent material constants are set in DATA statements. These include second- and third-order elastic constants, and the Bodner-Partom flow model parameters. Several sets of values remain in the listing with all but one deactivated with the comment character. These sets correspond to aluminum (Al), 2024 aluminum (2024), 6061-T6 aluminum (6061), graphite (C), graphite with the crystallographic z-axis along the fiber direction (CZ), diamond [C(D)], silica glass (SiO₂), and titanium (Ti). Additionally, there are the flow parameters for purely elastic response (EL). The constituent materials should be identified in the character variables "fiber" and "matrix," which are set in the final DATA statement.

Input:

name - Job name, up to 8 characters.

volfrac, aratf, aratc - fiber volume fraction, fiber aspect ratio (d_1/h_1), and RVE aspect ratio (D/H).

d0f, cnstf, cmstf, z0f, z1f - Bodner-Partom plasticity model parameters for fiber; D_0 , n , m , Z_0 , Z_1 , respectively.

d0m, cnstm, cmstm, z0m, z1m - Bodner-Partom plasticity model parameters for matrix; D_0 , n , m , Z_0 , Z_1 , respectively.

apply1, apply2, apply3 - Up to three strain or stress loading rates, depending on chosen load path. Units: s^{-1} or GPa/s.

rttn(3,3) and [rttn(1,1)] or [rttn(3,2) and rttn(1,3)] - Angles defining loading orientation for uniaxial strain or axial shear strain are entered into the rotation matrix elements and are converted in PATH into the appropriate rotation matrix. The two coordinate systems are the lab frame (X_i), in which the load is applied and the homogenized stresses and strains are given, and the composite frame (C_i). C_1 is in the fiber-direction. C_2 and C_3 need only form a right-handed system. Uniaxial strain is along the X_1 -direction. Transverse shear is

in the X_2 - X_3 plane. Axial shear is in the X_1 - X_3 plane unless it is reoriented by a rotation about the X_1 -axis. The angles entered as input are those between the C_i - and X_j -axes: *rttn*(3,3) initially holds the angle between the C_3 - and X_3 -axes; *rttn*(1,1) initially holds the angle between the C_1 - and X_1 -axes; *rttn*(3,2) initially holds the angle between the C_3 - and X_2 -axes; *rttn*(1,3) initially holds the angle between the C_1 - and X_3 -axes. If zero is entered for *rttn*(3,3), then only *rttn*(1,1) is requested additionally.

delt, *nsteps*, *iskip* - Time step in ms; number of steps to execute; number of time steps skipped between saving results for output. *iskip* is used to reduce the size of the output files.

crate, *dcr*, *knd* - These variables control automatic reduction of the time step as the subcell strains change from elastic to largely plastic. *crate* is the minimum elastic strain rate allowed in any subcell. The current (minimum) elastic strain rate among the four subcells (*erate*) is estimated as the difference of estimates of the maximum total strain rate of any subcell (*trtmax*) and the maximum plastic strain rate of any subcell (*prrtmax*). When *erate* falls below *crate*, the time step is halved and *crate* is multiplied by *dcr* (< 1.0). The time step is halved in this way up to *knd* times. Default values are *crate* = 0.001, *dcr* = 0.2, *knd* = 8.

ccvrg, *mxits* - When nonlinear elasticity is used, the convergence criterion, *ccvrg* (relative change in microvariable values), and the number of iterations allowed for reaching converged values, *mxits*, can be changed from their default values of 10^{-5} and 10, respectively.

AIRER: This is an error-trapping routine. Each subroutine is assigned a value of "noerr." If an error is detected, execution terminates after AIRER identifies the routine in which the error occurred (by its noerr value) and the approximate location of the error in that routine. Consulting the listing with this information often suffices to determine the cause of the problem.

CELLS: Subcell average stresses, macroscopic stress, strain, and plastic strain are computed here. The subcell stresses are obtained from the nonlinear elasticity constitutive relation.

EARL: Upon normal termination, this routine transforms the macroscopic stress and strain tensors from the composite coordinates back into the laboratory coordinates. The latter is the frame in which the applied load is defined.

ESTIM: Linear elasticity estimates of the microvariables are computed here. For applied strain, the microvariable values correspond to those of reference 9 generalized to orthorhombic symmetry (see Appendix E). The results for applied stress were not given previously, but are easily obtained (see Appendix E).

FLOW: This routine computes the plastic strain rate from the Bodner-Partom flow model. The predictor-corrector integration method ($\text{iflag} > 1$) has not been debugged.

MXINV: Square Matrix inversion routine. It works, but because it is borrowed from someone else's program, I have no information beyond that in the comments heading the routine.

NTIAL: Algebraic quantities are initialized here.

PATH: This routine increments the applied macroscopic stress or strain.

RESID: When nonlinear elasticity is used, one iteration of microvariable corrections for applied strain conditions are computed here.

DISER: When nonlinear elasticity is used, one iteration of microvariable corrections for applied stress conditions are computed here.

APPENDIX E. Analytic Solution of First-Order MoC with Linear Elasticity

Applied Macroscopic Strain Solution

The traction continuity conditions, Eqs. (45a, b), can be separated into four sets of equations (time derivatives will be omitted):

- (1) The four equations involving normal stress components. These determine the eight microvariables $\phi_2^{\alpha\gamma}$ and $\psi_3^{\alpha\gamma}$.
- (2) The two equations involving the stress component S_{12} . These determine the four microvariables $\phi_1^{\alpha\gamma}$.
- (3) The two equations involving the stress component S_{13} . These determine the four microvariables $\psi_1^{\alpha\gamma}$.
- (4) The three independent equations involving the stress component S_{23} . These determine the four microvariable combinations $\phi_3^{\alpha\gamma} + \psi_2^{\alpha\gamma}$.

The four equations involving normal stress components are

$$S_{22}^{11} = S_{22}^{21}, \quad S_{22}^{12} = S_{22}^{22}, \quad S_{33}^{11} = S_{33}^{12}, \quad \text{and} \quad S_{33}^{21} = S_{33}^{22}. \quad (\text{E1})$$

Substituting from the linear elastic constitutive relations, Eqs. (C16) and (C17) in Appendix C, and using displacement continuity, Eqs. (39b), (40b), and (41), in the form

$$\phi_2^{21} = \frac{1}{d_2} (D\bar{\epsilon}_2 - d_1 \phi_2^{11}), \quad \phi_2^{12} = \frac{1}{d_1} (D\bar{\epsilon}_2 - d_2 \phi_2^{22}), \quad (\text{E2a,b})$$

$$\psi_3^{21} = \frac{1}{h_1} (D\bar{\epsilon}_3 - h_2 \psi_3^{22}), \quad \psi_3^{12} = \frac{1}{h_2} (D\bar{\epsilon}_3 - h_1 \psi_3^{11}), \quad (\text{E2c,d})$$

provides four simultaneous linear equations for the remaining microvariables. The solution is

$$\begin{pmatrix} \phi_2^{11} \\ \phi_2^{22} \\ \psi_3^{11} \\ \psi_3^{22} \end{pmatrix} = (\underline{\underline{M}}_1)^{-1} \left[\underline{\underline{M}}_2 \begin{pmatrix} \bar{\epsilon}_1 \\ \bar{\epsilon}_2 \\ \bar{\epsilon}_3 \end{pmatrix} + \underline{\underline{M}}_3 \right], \quad (\text{E3})$$

$$(\text{rank:} \quad \quad \quad 4 \times 4 \quad \quad 4 \times 3 \quad \quad 4 \times 1)$$

where

$$\underline{\underline{M}}_1 \equiv \begin{bmatrix} C_{22}^{11} + \frac{d_1}{d_2} C_{22}^{21} & 0 & C_{23}^{11} & \frac{h_2}{h_1} C_{23}^{21} \\ 0 & C_{22}^{22} + \frac{d_2}{d_1} C_{22}^{12} & \frac{h_1}{h_2} C_{23}^{12} & C_{33}^{22} \\ C_{23}^{11} & \frac{d_2}{d_1} C_{23}^{12} & C_{33}^{11} + \frac{h_1}{h_2} C_{33}^{12} & 0 \\ \frac{d_1}{d_2} C_{23}^{21} & C_{23}^{22} & 0 & C_{33}^{22} + \frac{h_2}{h_1} C_{33}^{21} \end{bmatrix},$$

$$\underline{\underline{M}}_2 \equiv \begin{bmatrix} C_{12}^{21} - C_{12}^{11} & \frac{D}{d_2} C_{22}^{21} & \frac{H}{h_1} C_{23}^{21} \\ C_{12}^{12} - C_{12}^{22} & \frac{D}{d_1} C_{22}^{12} & \frac{H}{h_2} C_{23}^{12} \\ C_{13}^{12} - C_{13}^{11} & \frac{D}{d_1} C_{23}^{12} & \frac{H}{h_2} C_{33}^{12} \\ C_{13}^{21} - C_{13}^{22} & \frac{D}{d_2} C_{23}^{21} & \frac{H}{h_1} C_{33}^{21} \end{bmatrix},$$

and

$$\underline{\underline{M}}_3 \equiv \begin{bmatrix} C_{12}^{11} L_1^{11} + C_{22}^{11} L_2^{11} + C_{23}^{11} L_3^{11} - C_{12}^{21} L_1^{21} - C_{22}^{21} L_2^{21} - C_{23}^{21} L_3^{21} \\ C_{12}^{22} L_1^{22} + C_{22}^{22} L_2^{22} + C_{23}^{22} L_3^{22} - C_{12}^{12} L_1^{12} - C_{22}^{12} L_2^{12} - C_{23}^{12} L_3^{12} \\ C_{13}^{11} L_1^{11} + C_{23}^{11} L_2^{11} + C_{33}^{11} L_3^{11} - C_{13}^{12} L_1^{12} - C_{23}^{12} L_2^{12} - C_{33}^{12} L_3^{12} \\ C_{13}^{22} L_1^{22} + C_{23}^{22} L_2^{22} + C_{33}^{22} L_3^{22} - C_{13}^{21} L_1^{21} - C_{23}^{21} L_2^{21} - C_{33}^{21} L_3^{21} \end{bmatrix}$$

Upon obtaining the other four microvariables from Eqs. (E2a through d), the solution agrees with Eq. (23) of reference 9 for the cases treated there.

The equations involving the (12) stress components are

$$S_{12}^{11} = S_{12}^{21} \quad \text{and} \quad S_{12}^{12} = S_{12}^{22} . \quad (\text{E4})$$

Displacement continuity, Eqs. (39b) and (41), provide

$$\phi_1^{21} = \frac{1}{d_2} (D\bar{w}_{1,2} - d_1\phi_1^{11}) \quad \text{and} \quad \phi_1^{12} = \frac{1}{d_1} (D\bar{w}_{1,2} - d_2\phi_1^{22}) \quad (\text{E5a,b})$$

Substituting into Eqs. (E4) from Eqs. (C20) and (E5) leads to the solutions

$$\phi_1^{11} = \frac{d_2 \bar{w}_{2,1} (C_{66}^{21} - C_{66}^{11}) + D \bar{w}_{1,2} C_{66}^{21} + 2d_2 (C_{66}^{11} L_6^{11} - C_{66}^{21} L_6^{21})}{d_1 C_{66}^{21} + d_2 C_{66}^{11}} , \quad (\text{E6a})$$

and

$$\phi_1^{22} = \frac{d_1 \bar{w}_{2,1} (C_{66}^{12} - C_{66}^{22}) + D \bar{w}_{1,2} C_{66}^{12} + 2d_1 (C_{66}^{22} L_6^{22} - C_{66}^{12} L_6^{12})}{d_1 C_{66}^{22} + d_2 C_{66}^{12}} . \quad (\text{E6b})$$

These results agree with Eq. (29) of reference 9 for the cases treated there. The difference of matrix elastic constants $(C_{66}^{12} - C_{66}^{22})$ does not vanish when either a damage model or strain-dependent elastic constants are used.

The results for the (13) stress components are analogous to Eqs. (E4) through (E6):

$$S_{13}^{11} = S_{13}^{12} \quad \text{and} \quad S_{13}^{21} = S_{13}^{22} . \quad (\text{E7})$$

Displacement continuity, Eqs. (40b) and (41), provide

$$\psi_1^{21} = \frac{1}{h_1} (H\bar{w}_{1,3} - h_2\psi_1^{22}) \quad \text{and} \quad \psi_1^{12} = \frac{1}{h_2} (H\bar{w}_{1,3} - h_1\psi_1^{11}) . \quad (\text{E8a,b})$$

Substituting into Eqs. (E7) from Eqs. (C19) and (E8a and b) leads to the solutions

$$\psi_1^{11} = \frac{h_2 \bar{w}_{3,1} (C_{55}^{12} - C_{55}^{11}) + H \bar{w}_{1,3} C_{55}^{12} + 2h_2 (C_{55}^{11} L_5^{11} - C_{55}^{12} L_5^{12})}{h_1 C_{55}^{12} + h_2 C_{55}^{11}}, \quad (E9a)$$

and

$$\psi_1^{22} = \frac{h_1 \bar{w}_{3,1} (C_{55}^{21} - C_{55}^{22}) + H \bar{w}_{1,3} C_{55}^{21} + 2h_1 (C_{55}^{22} L_5^{22} - C_{55}^{21} L_5^{21})}{h_1 C_{55}^{22} + h_2 C_{55}^{21}}. \quad (E9b)$$

Finally, the four microvariable combinations $\phi_3^{\alpha\gamma} + \psi_2^{\alpha\gamma}$ are determined from Eq. (46) and any three of the traction continuity conditions involving the (23) stress components. We choose to use

$$S_{23}^{11} = S_{23}^{21}, \quad S_{23}^{21} = S_{23}^{22}, \quad \text{and} \quad S_{23}^{12} = S_{23}^{22}. \quad (E10)$$

The expression for ζ^{12} obtained from Eq. (46),

$$\zeta^{12} = [DH \bar{\epsilon}_4 - (d_1 h_1 \zeta^{11} + d_2 h_1 \zeta^{21} + d_2 h_2 \zeta^{22})] / d_1 h_2, \quad (E11)$$

is substituted into the last equation of Eq. (E10). The resulting solution consists of Eq. (E11) and

$$\begin{pmatrix} \zeta^{11} \\ \zeta^{21} \\ \zeta^{22} \end{pmatrix} = \begin{pmatrix} C_{44}^{11} & -C_{44}^{21} & 0 \\ 0 & -C_{44}^{21} & C_{44}^{22} \\ \frac{h_1}{h_2} C_{44}^{12} & \frac{d_2 h_1}{d_1 h_2} C_{44}^{12} & C_{44}^{22} + \frac{d_2}{d_1} C_{44}^{12} \end{pmatrix}^{-1} \begin{pmatrix} C_{44}^{11} L_4^{11} - C_{44}^{21} L_4^{21} \\ C_{44}^{22} L_4^{22} - C_{44}^{21} L_4^{21} \\ C_{44}^{22} L_4^{22} + C_{44}^{12} \left(\frac{DH}{d_1 h_2} \bar{\epsilon}_4 - L_4^{21} \right) \end{pmatrix}. \quad (E12)$$

Applied Macroscopic Normal Stress Solution

The four stress continuity equations, Eq. (E1), four displacement continuity equations, Eqs. (E2a through b), and the three macroscopic normal stress definitions, Eq. (47) with $f^{\alpha\gamma} = S^{\alpha\gamma}$ and $\bar{f} = \bar{\sigma}$, provide eleven equations that determine eight microvariables and the three macroscopic normal strain components. Combining the macroscopic normal stress definitions with Eq. (E1), two of the macroscopic stress components reduce to

$$H \bar{\sigma}_{22} = h_1 S_2^{11} + h_2 S_2^{22}, \quad (\text{E13a})$$

and

$$D \bar{\sigma}_{33} = d_1 S_3^{11} + d_2 S_3^{22}. \quad (\text{E13b})$$

Upon substituting from the linear elastic constitutive relations, Eqs. (C15) through (C17), and using displacement continuity, Eqs. (E2a through b), the macroscopic stress definitions and stress continuity equations become

$$[\bar{\epsilon}_1, \bar{\epsilon}_2, \bar{\epsilon}_2, \phi_2^{11}, \phi_2^{22}, \psi_3^{11}, \psi_3^{22}]^T = (\underline{\underline{M}}_4)^{-1} \underline{\underline{B}}, \quad (\text{E14})$$

$$(\text{rank:} \quad \quad \quad 7 \times 7 \quad 7 \times 1)$$

where

$$\underline{\underline{M}}_4 \equiv \begin{bmatrix} C_{12}^{11} - C_{12}^{21} & -\frac{D}{d_2} C_{22}^{21} & -\frac{H}{h_1} C_{23}^{21} & C_{22}^{11} + \frac{d_1}{d_2} C_{22}^{21} & 0 & C_{23}^{11} & \frac{h_2}{h_1} C_{23}^{21} \\ C_{12}^{22} - C_{12}^{12} & -\frac{D}{d_1} C_{22}^{12} & -\frac{H}{h_2} C_{23}^{12} & 0 & C_{22}^{22} + \frac{d_2}{d_1} C_{22}^{12} & \frac{h_1}{h_2} C_{23}^{12} & C_{23}^{22} \\ C_{13}^{11} - C_{13}^{12} & -\frac{D}{d_1} C_{23}^{12} & -\frac{H}{h_2} C_{33}^{12} & C_{23}^{11} & \frac{d_2}{d_1} C_{23}^{12} & C_{33}^{11} + \frac{h_1}{h_2} C_{33}^{12} & 0 \\ C_{13}^{22} - C_{13}^{21} & \frac{D}{d_2} C_{23}^{21} & \frac{H}{h_1} C_{33}^{21} & \frac{d_1}{d_2} C_{23}^{21} & C_{23}^{22} & 0 & C_{33}^{22} + \frac{h_2}{h_1} C_{33}^{21} \\ C_{12}^{11} + \frac{h_2}{h_1} C_{12}^{22} & 0 & 0 & C_{22}^{11} & \frac{h_2}{h_1} C_{22}^{22} & C_{23}^{11} & \frac{h_2}{h_1} C_{23}^{22} \\ C_{13}^{11} + \frac{d_2}{d_1} C_{13}^{22} & 0 & 0 & C_{23}^{11} & \frac{d_2}{d_1} C_{23}^{22} & C_{33}^{11} & \frac{d_2}{d_1} C_{33}^{22} \\ M_{4,71} & D(C_{12}^{21} h_1 + C_{12}^{12} h_2) & H(C_{13}^{21} d_2 + C_{13}^{12} d_1) & d_1 h_1 (C_{12}^{11} - C_{12}^{21}) & d_2 h_2 (C_{12}^{22} - C_{12}^{12}) & d_1 h_1 (C_{13}^{11} - C_{13}^{12}) & d_2 h_2 (C_{13}^{22} - C_{13}^{21}) \end{bmatrix}$$

with $M_{4,71} = d_1 h_1 C_{11}^{11} + d_2 h_1 C_{11}^{21} + d_1 h_2 C_{11}^{12} + d_2 h_2 C_{11}^{22}$, and

$$\underline{\underline{B}} \equiv \begin{bmatrix} C_{12}^{11}L_1^{11} + C_{22}^{11}L_2^{11} + C_{23}^{11}L_3^{11} - C_{12}^{21}L_1^{21} + C_{22}^{21}L_2^{21} - C_{23}^{21}L_3^{21} \\ C_{12}^{22}L_1^{22} + C_{22}^{22}L_2^{22} + C_{23}^{22}L_3^{22} - C_{12}^{12}L_1^{12} + C_{22}^{12}L_2^{12} - C_{23}^{12}L_3^{12} \\ C_{13}^{11}L_1^{11} + C_{23}^{11}L_2^{11} + C_{33}^{11}L_3^{11} - C_{13}^{12}L_1^{12} + C_{23}^{12}L_2^{12} - C_{33}^{12}L_3^{12} \\ C_{13}^{22}L_1^{22} + C_{23}^{22}L_2^{22} + C_{33}^{22}L_3^{22} - C_{13}^{21}L_1^{21} + C_{23}^{21}L_2^{21} - C_{33}^{21}L_3^{21} \\ \frac{H}{h_1}\bar{\sigma}_2 + C_{12}^{11}L_1^{11} + C_{22}^{11}L_2^{11} + C_{23}^{11}L_3^{11} + \frac{h_2}{h_1}(C_{12}^{22}L_1^{22} + C_{22}^{22}L_2^{22} + C_{23}^{22}L_3^{22}) \\ \frac{D}{d_1}\bar{\sigma}_3 + C_{13}^{11}L_1^{11} + C_{23}^{11}L_2^{11} + C_{33}^{11}L_3^{11} + \frac{d_2}{d_1}(C_{13}^{22}L_1^{22} + C_{23}^{22}L_2^{22} + C_{33}^{22}L_3^{22}) \end{bmatrix},$$

B_7

where

$$B_7 = DH \bar{\sigma}_1 + d_1 h_1 (C_{11}^{11}L_1^{11} + C_{12}^{11}L_2^{11} + C_{13}^{11}L_3^{11}) + d_2 h_1 (C_{11}^{21}L_1^{21} + C_{12}^{21}L_2^{21} + C_{13}^{21}L_3^{21}) \\ + d_1 h_2 (C_{11}^{12}L_1^{12} + C_{12}^{12}L_2^{12} + C_{13}^{12}L_3^{12}) + d_2 h_2 (C_{11}^{22}L_1^{22} + C_{12}^{22}L_2^{22} + C_{13}^{22}L_3^{22}).$$

The remaining four normal stress microvariables are obtained from Eqs. (E2a –b).

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