International Journal for Computational Civil and Structural Engineering, Vol 1, pp. 64–78 (2000)

Embedding a Micromechanical Law in the Continuum Formulation: A Multiscale Approach Applied to Discontinuous Solutions

Krishna Garikipati and Thomas J. R. Hughes

Division of Mechanics and Computation Stanford University, Stanford, California

* Address correspondence to: Division of Mechanics and Computation, Stanford University, Stanford, CA 94305.

ABSTRACT: The framework of multiscale analysis has been applied to strain localization problems. It is now extended to the case of strong discontinuities. This term describes displacement fields that possess a discontinuous component. The analysis of discontinuous solutions arising in one-dimensional, rate-independent plasticity is revisited. The resulting formulation is treated as a microstructural model that is sought to be embedded in the standard, macromechanical continuum framework. In a neighborhood of the discontinuity, one can identify coarse and fine scale fields such that the discontinuous component is contained in the latter. With this decomposition as a basis, multiscale analysis is used as a vehicle to effect the desired embedding. The features of the strong discontinuities model for strain-softening solids are shown to be retained in the resulting multiscale model.

1 INTRODUCTION

Discontinuous solutions are admissible under certain conditions in inviscid solids that display nonlinear, inelastic material response. Such solutions involve localized strains. Typically, strain softening is associated with the constitutive equations. Examples include softening plasticity and continuum damage degradation. We begin by reviewing the literature on strain localization for inviscid materials.

Some of the earliest investigations date back to Hadamard [1] and the study of propagating discontinuities. In classical rigid plastic theory, the problem posed in terms of stress is hyperbolic. The characteristics coincide with lines of plastic flow termed slip lines (see Geiringer [2]). Traditionally, the analysis of strain localization problems has been carried out in the framework of the theory of plasticity; more recently, theories of continuum damage degradation have been used (see Willam [3]). The strains are typically assumed to be localized over a region of finite measure. The displacement field has a high gradient over this region, but is continuous, and the strain field is discontinuous. Such fields are termed "weak discontinuities." They were considered by Thomas [4] under the plane stress condition in uniaxial tension. Necessary conditions were derived for the presence of the assumed deformation patterns and, for the von Mises and Tresca yield criteria, the angle of inclination of the localization band was obtained. The analysis is carried forward in Hill [5] and Mandel [6] in the framework first explored by Hadamard.[1] An analysis in the context of bifurcations in the plane tension test is carried out in Hill and Hutchinson.[7] Detailed investigations of strain localization for various plasticity models appear in Rice [8] and Rice and Rudnicki [9] for departures from normality in the flow rule. A comprehensive review from the micromechanical standpoint is presented in Asaro.[10] Other studies of note are Ottosen and Runesson [11] and Bigoni and Zaccaria.[12]

A central feature of the investigations listed above is that the loss of strong ellipticity of the continuum tangent appears as a necessary condition for strain localization. This is a well-known and classical condition (see standard texts such as Graff [13] or Marsden and Hughes [14] and corresponds to vanishing wave speeds when the dynamic problem is considered. The assumption of weak discontinuities in the analyses above introduces a length scale associated with the finite region of strain localization. The classical continuum theory for inviscid solids does not possess such a length. Furthermore, for a strain-softening continuum, on assuming the presence of such a length scale and considering the limiting case as it tends to zero, the solutions arrived at are nonphysical. In particular, the dissipation is found to vanish. This is interpreted

1524-5845/2000/$5

as a manifestation of the ill-posedness of the strain-softening continuum for rate-independent solids. Nonunique solutions are obtained in such a setting.

For plasticity, a significant body of work is available on existence, regularity, and uniqueness of solutions. We recall some of these results here. While the existence of a stress field satisfying the plasticity constraint, the governing differential equations, and boundary conditions can be proven, a corresponding strain field cannot be found in complete generality (Duvaut and Lions [15]). For hardening plasticity, when normality applies, a strain field corresponding to the stress can be found by inverting the tangent operator (Johnson [16]). Existence results in a variational setting are provided in Johnson [17] and Anzellotti and Giaquinta.[18] It was shown by Matthies et al.[19] that, for classical plasticity, the correct space for the displacement field is the so-called space of bounded deformation. This space admits discontinuous fields (strong discontinuities). The corresponding strains are bounded measures, a set that includes Dirac delta functions. With this work as a point of departure, Simo et al.[20] analyzed classical models of softening plasticity and continuum damage degradation assuming the presence of discontinuous displacements. The analysis is carried out in the framework of the theory of distributions. It is demonstrated that meaningful results can be obtained for the stress, plastic variables, and dissipation. Furthermore, the loss of strong ellipticity again appears as a necessary condition and, importantly, an evolution equation emerges for the discontinuous displacement component in relation to the stress. Extensions of this work appear in Simo, and Qliver [21], Armero and Garikipati [22, 23] (where finite strain plasticity is treated), and Oliver.[24] The approach incorporating strong discontinuities treats the limiting problem of a vanishing localization width. It is of crucial importance that the problem remains well posed when formulated in the distributional framework.

The ill-posedness of the classical strain-softening continuum leads to highly mesh-dependent solutions when the standard finite element method is applied. A number of alternative formulations have been proposed to regularize the problem — see Bazant [25] and Garikipati and Hughes [26] for a review. In contrast, a crucial advantage of the formulation based on strong discontinuities is that the problem is rendered well posed and, therefore, numerical solution based on it do not display spurious mesh dependence.

We now provide the motivation for the present work. Garikipati and Hughes [26] addressed the problem of strain localization by recognizing the inherent length scales and developing a model that accounts fully for the fine scale. For an inviscid strain-softening continuum, given a particular fine scale structure, the model then results in mesh-invariant solutions. Furthermore the regularizing effects of several alternative formulations are recovered. The framework in which these properties were demonstrated involved a localization band of finite width, achieved by a suitable perturbation of the material properties. However, the study did not purport to advocate the use of finite widths for strain localization. The issue of well-posedness of the problem when the width tends to zero was left unaddressed; but, it was stated that the problem of strong discontinuities could also be placed in a multiscale framework and a model built for it. It is to this task that attention is now turned. In the presence of strong discontinuities, the region of localized strain is now replaced by a surface of zero measure. In the neighborhood of this discontinuity surface, a smooth approximation to the actual solution can be identified and is referred to as the coarse scale. The difference between the total solution and the coarse field is the fine scale which includes the discontinuous component. As in Garikipati and Hughes,[26] the aim is to develop, for the coarse scale, a model that contains the effect of the fine scale field. *Importantly, the philosophy involves the treatment of the strong discontinuities formulation as a given microstructural model that we seek to embed in a standard macromechanical framework.*

The rest of the article is organized as follows. A review of the model incorporating strong discontinuities is presented in Section 2. Section 3 develops the multiscale model. The computational formulation is presented in Section 4, numerical simulations in Section 5, and a closure in Section 6.

2 THE STRONG DISCONTINUITIES FORMULATION

This section outlines the analysis of a one-dimensional plasticity model for the case of a solution that possess strong discontinuities. The development follows that of Simo et al.[20] and Armero and Garikipati.[23]

Consider a body, in our case, an open set in $\mathbb{R}^2$, subjected to simple shear as shown in Figure 1. We model it as a one-dimensional problem, where the

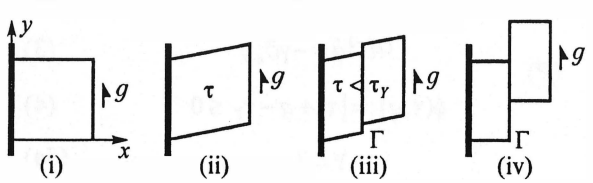

Figure 1. Shear problem with discontinuity surface Γ.

variables of interest are the shear stress τ, the vertical displacement u and the shear strain $\partial u/\partial x$. The domain of interest is now an open interval on the horizontal axis denoted $\Omega \subset \mathbb{R}^1$. The material is assumed to be elastoplastic with initial yield stress τ_Y, and follows a linear softening law after yielding.

The evolution of the problem, depicted in Figure 1, consists of the following stages: (i) the undeformed configuration; (ii) under an imposed tip displacement g, the block deforms and develops shear stress τ; (iii) plastic response begins at a stress, τ_Y, following which the displacement field in the material develops a discontinuity along the line Γ; and (iv) the strain is localized on Γ and strain softening sets in, allowing the material outside Γ to relax elastically. In the final state, the body has a displacement field consisting only of the discontinuity at Γ. Figure 2 shows the corresponding evolution of stress.

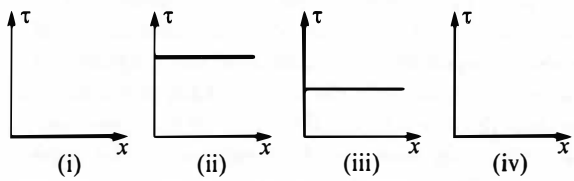

Figure 2. Evolution of stress for the idealized one-dimensional problem.

It this setting, made special by the discontinuous displacement, the following issues arise:

1. Implications for the stress at the discontinuity Γ.
2. The form taken by the total and inelastic strains in the presence of a discontinuous displacement.
3. An interpretation of the softening law.
4. A relation describing material response following the development of the discontinuity.

2.1 Plastic Constitutive Equations

The constitutive model (i.e., the set of relations governing one-dimensional, rate-independent plasticity) is introduced next:

$$(P)\quad \begin{aligned} &\dot{\tau} = G(\dot{u}_{,x} - \dot{\varepsilon}^p) && (1)\\ &\dot{\varepsilon}^p = \gamma \partial_\tau \phi && (2)\\ &\mathcal{H}^{-1}\dot{q} = -\gamma \partial_q \phi && (3)\\ &\phi(\tau, q) := |\tau| + q - \tau_Y \le 0 && (4)\\ &\gamma \ge 0 && (5a)\\ &\phi(\tau, q) \le 0 && (5b)\\ &\gamma\phi = 0 && (5c)\\ &\gamma\dot{\phi}(\tau, q) = 0 && (6) \end{aligned}$$

Here, G is the shear modulus, ε^p is the plastic strain, γ is a plastic multiplier, and q is a stresslike variable. The softening law is given by equation (3), with $\mathcal{H} < 0$ being the softening parameter. The constraint $\phi(\tau, q) \le 0$ defines the yield condition. The Kuhn–Tucker loading/unloading conditions are equations (5). For instantaneously evolving plastic flow ($\gamma > 0$), $\dot{\phi}(\tau, q) = 0$; that is, equation (6) is the plastic consistency condition. The constitutive relations above, between τ and u, hold in the following strong form of the problem of stress equilibrium in which we find

$$\begin{aligned} u &\in \mathcal{S} = \{u \mid u = g \quad \text{on} \quad \partial\Omega_u\}\\ \tau &\in \mathcal{T} = \{\tau \mid \tau = t \quad \text{on} \quad \partial\Omega_t\} \end{aligned} \tag{7}$$

where $\overline{\partial\Omega} = \overline{\partial\Omega_u \cup \partial\Omega_t}$, $\partial\Omega_u \cap \partial\Omega_t = \varnothing$, such that

$$\frac{\partial \tau}{\partial x} + f = 0 \quad \text{in} \quad \Omega \tag{8}$$

where $f(x)$ is a given function.

2.2 Discontinuous Displacement Fields

Consider a displacement field that admits a discontinuity located at Γ.

$$u(x,t) = \underbrace{\hat{u}(x,t)}_{\text{continuous}} + \underbrace{[u](t) H_\Gamma(x)}_{\text{discontinuous}} \tag{9}$$

where, H_Γ is the Heaviside function defined as

$$H_\Gamma(x) = \begin{cases} 0: & x \in (-\infty, \Gamma) \\ 1: & x \in [\Gamma, \infty) \end{cases} \tag{10}$$

Then, the displacement rate follows as,

$$\dot{u}(x,t) = \dot{\hat{u}}(x,t) + [\dot{u}](t) H_\Gamma(x) \tag{11}$$

The derivative of $H_\Gamma(x)$ with respect to x is the Dirac delta function $\delta_\Gamma(x)$. This result follows by adopting a distributional view of H_Γ and working within this framework to define its derivative. The strain rate is written as follows:

$$\dot{u}_{,x}(x,t) = \underbrace{\dot{\hat{u}}_{,x}(x,t)}_{\text{regular}} + \underbrace{[\dot{u}](t)\delta_\Gamma(x)}_{\text{singular}} \tag{12}$$

In the distributional framework, the total strain rate $\dot{u}_{,x}$ has regular and singular components, as indicated above. The reader is directed to standard works such as Stakgold[27] for details from the theory of distributions. Formal definitions of regular and singular distributions are also provided there. For our purposes, it will suffice to refer to any expression with a Dirac delta function as being singular. All others are regular.

Remark 1. *In general,* Γ *is a set of zero measure with dimension* $n-1$ *for a problem posed in* $\mathbb{R}^n$. *Put differently, it is an* $(n-1)$*-dimensional hypersurface in* $\mathbb{R}^n$.

2.3 Stress and Plastic Multiplier

For the problem under consideration, assuming that f is a regular distribution in a neighborhood of Γ, it follows from equation (8) that τ is continuous on Ω. A fundamental assumption is now introduced:

Assumption 1. *The continuum model remains applicable in the presence of the discontinuous displacement.*

This implies that the stress remains continuous in the presence of the discontinuous component; that is, $[\![\tau]\!]|_\Gamma = 0$, and leads to the conclusion that the stress rate is regular (see Armero and Garikipati[23]). From equations (1), (2), (4), and (12), the stress rate can be written as follows:

$$\underbrace{\dot{\tau}|_\Gamma}_{\text{regular}} = G[\underbrace{\dot{\hat{u}}_{,x}}_{\text{regular}} + \underbrace{[\![\dot{u}]\!]\delta_\Gamma}_{\text{singular}} - \gamma\,\mathrm{sign}(\tau)] \tag{13}$$

where, $\partial\phi/\partial\tau = \mathrm{sign}(\tau)$ has been used. By comparing the regular and singular terms in equation (13), we see that γ must be a singular distribution. This is written as follows:

$$\gamma = \hat{\gamma} + \gamma_\delta\delta_\Gamma,\ \ \hat{\gamma} \geq 0,\ \ \gamma_\delta \geq 0 \tag{14}$$

where $\hat{\gamma}$ is regular, and the nonnegativity of $\hat{\gamma}$ and γ_δ follows from the decomposition of equations (14) and (5a). Assuming that $\hat{\gamma}$ vanishes, the plastic flow is localized to the discontinuity surface Γ. Substituting γ from equation (14) into (13), it follows that the nonzero part of the plastic multiplier is

$$\gamma_\delta = [\![\dot{u}]\!]\mathrm{sign}(\tau) \tag{15}$$

In light of the singular distributional from for the plastic multiplier, the softening law is examined.

2.4 The Softening Law

Turning to the yield criterion in equation (4), we observe that it imposes a pointwise bound on $|\tau|$ and q. If we invoke Assumption 1, it follows that this bound remains valid in the presence of the discontinuity. From the conclusion that $\dot{\tau}$ is regular and the consistency condition, it follows that $\dot{q}$ is a regular distribution. The softening law in equation (3) is

$$\mathcal{H}^{-1}\underbrace{\dot{q}}_{\text{regular}} = -\gamma\partial_q\phi = \underbrace{-\gamma_\delta\delta_\Gamma}_{\text{singular}} \tag{16}$$

From the relation above, it follows that the softening parameter must have the form

$$\mathcal{H}^{-1} = \overline{\mathcal{H}}^{-1}\delta_\Gamma \tag{17}$$

that is, its reciprocal is a singular distribution. Physically, plastic softening is also limited to the discontinuity surface Γ.

Remark 2. *The form taken by the softening parameter in equation (17) results in a regularization of the problem (see Simo et al.*[20] *for details).*

2.5 Evolution of the Displacement Jump

From plastic consistency, $\dot{\phi}(\tau, q) = 0$, it follows that

$$\mathrm{sign}(\tau)\dot{\tau} + \dot{q} = 0 \tag{18}$$

On substituting equation (17) into (16) and evaluating the expression at Γ, we have

$$\dot{q}|_\Gamma = -\overline{\mathcal{H}}\gamma_\delta \tag{19}$$

From equations (15), (18), and (19), the following evolution law for $[\![u]\!]$ emerges:

$$[\![\dot{u}]\!] = \overline{\mathcal{H}}^{-1}\dot{\tau}|_\Gamma \tag{20}$$

This law is the constitutive relation that governs the evolution of the discontinuous displacement component.

Remark 3. *The relation in equation (20) takes on the form of a stress displacement law. This is similar to the constitutive relation specified in the approach of Hillerborg and coworkers.*[28, 29]

2.6 A Micromechanical Law

From equations (14) and (15), it follows that

$$[\![\dot{u}]\!] = |[\![\dot{u}]\!]|\mathrm{sign}(\tau) \tag{21}$$

Combining equations (15), (19), and (21) gives

$$\dot{q}|_{\Gamma} = -\overline{\mathcal{H}}|[\![\dot{u}]\!]| \tag{22}$$

and, letting the value of q at the onset of the discontinuity be $q = 0$, we have

$$q|_{\Gamma} = -\overline{\mathcal{H}}|[\![u]\!]| \tag{23}$$

Here, attention is drawn to the failure of q to evolve in the absence of localized plastic flow. Correspondingly, there is no contraction (in stress space) of the region of admissible stress [see equations (4) and (22)].

The analysis above is now summarized and posed as a micromechanical model on $\Gamma \subset \Omega$:

$$\psi(\tau,[\![u]\!]) = |\tau| - \left(\tau_Y + \overline{\mathcal{H}}|[\![u]\!]|\right) \le 0 \tag{24}$$

$$|[\![\dot{u}]\!]| = \overline{\mathcal{H}}^{-1}(\dot{\tau}\,\mathrm{sign}[\tau])|_{\Gamma}, \quad \overline{\mathcal{H}} < 0 \tag{25}$$

$$(M) \qquad \psi|[\![\dot{u}]\!]| = 0 \tag{26}$$

$$\dot{\psi}|[\![\dot{u}]\!]| = 0 \tag{27}$$

Equation (24) follows by combining equations (4) and (23) and can be viewed as the yield condition for the micromechanical model. Equation (25) is obtained by combining equations (18) and (22). It represents the flow rule for evolution of the magnitude of the discontinuous displacement, $|[\![u]\!]|$. Equation (26) emerges from equations (15) and (21) combined with the Kuhn–Tucker condition in equation (5c) and has the interpretation of the loading/unloading condition for this model. Finally, equation (27) is obtained from equations (15) and (21) combined with the consistency condition, equation (6). Clearly, it serves as the consistency condition for the micromechanical model.

It is instructive to compare the micromechanical model in equations (24) to (27) with the plasticity model in equations (1) to (6). For this purpose, the following observations are useful:

1. For plastic flow, the consistency condition, the yield condition, and the flow rule [equations (6), (4), and (3), respectively] give

$$\begin{aligned} &\dot{\phi}(\tau,q) = 0 \\ &\Rightarrow \dot{\tau}\,\mathrm{sign}(\tau) = -\dot{q} \\ &\Rightarrow \dot{\tau}\,\mathrm{sign}(\tau) = \mathcal{H}\gamma \quad \text{in} \quad \Omega\backslash\Gamma \end{aligned} \tag{28}$$

2. From equations (23) and (24) the yield function in equations (24) to (27) can be rewritten as follows:

$$\overline{\psi}(\tau,q) = |\tau| + q - \tau_Y \le 0 \tag{29}$$

Now, with equations (4), (28), (5), and (6) describing the plasticity model in $\Omega\backslash\Gamma$, and equations (29), (25), (26), and (27) describing the micromechanical model on Γ, it is seen that the two models are essentially identical in form:

Model	(P)	(M)
Yield function	$\phi(\tau,q) = \lvert\tau\rvert + q - \tau_Y$	$\overline{\psi}(\tau,q) = \lvert\tau\rvert + q - \tau_Y$
Flow rule	$\dot{\tau}\,\mathrm{sign}(\tau) = \mathcal{H}\gamma$	$\dot{\tau}\,\mathrm{sign}(\tau) = \overline{\mathcal{H}}\lvert[\![\dot{u}]\!]\rvert$
Kuhn–Tucker	$\gamma \ge 0,\ \phi(\tau,q) \le 0,\ \gamma\phi = 0$	$\lvert[\![\dot{u}]\!]\rvert \ge 0,\ \overline{\psi}(\tau,q) \le 0,\ \lvert[\![\dot{u}]\!]\rvert\,\overline{\psi} = 0$
Consistency	$\gamma\dot{\phi} = 0$	$\lvert[\![\dot{u}]\!]\rvert\,\dot{\overline{\psi}} = 0$

This micromechanical interpretation of the strong discontinuities model will form the basis for its treatment in the multiscale framework.

Remark 4. *The missing ingredient in the development above is a condition for the appearance of the discontinuous displacement. For the present one-dimensional case, with softening, the condition that triggers the discontinuous component is merely the onset of plastic flow.*

3 STRONG DISCONTINUITIES IN A MULTISCALE FRAMEWORK

In setting the stage for the application of the multiscale framework to the model of strong discontinuities, we have posed the latter as a micromechanical model (in higher dimensions, this derived micromechanical model corresponds to the Schmid law of crystal plasticity). The development that follows aims at incorporating this model in the standard (macromechanical) continuum framework.

3.1 The Multiscale Decomposition

We begin by choosing a subdomain Ω_e, open in Ω, such that $\Omega_e \subset \Omega$, $\Omega_e \ne \Omega$. Furthermore, the subdomain Ω_e is chosen such that the discontinuity introduced in Section 2 satisfies $\Gamma \in \Omega_e$ and separates Ω_e into open sets Ω_e^- and Ω_e^+, where $\Omega_e = \Omega_e^- \cup \Omega_e^+ \cup \Gamma$, and $\Omega_e^- \cap \Gamma = \Omega_e^- \cap \Omega_e^+ = \Omega_e^+ \cap \Gamma = \varnothing$. Consider the weak form, (W),

Find $u \in \mathcal{S} = \{u | u = g \text{ on } \partial\Omega_u\}$, and σ satisfying (P) in $\Omega \backslash \Gamma$ such that

$$(W) \qquad \int_{\Omega} w_{,x}\, \sigma\, dV - \int_{\Omega} w f\, dV - \int_{\partial\Omega_t} w t\, dS = 0 \tag{30}$$

where, w denotes the weighting function:

$$w \in \mathcal{V} = \{w | w = 0 \text{ on } \partial\Omega_u\} \tag{31}$$

In a change of notation, the stress has been written as σ in the weak form above since, in what follows, it is desired to reserve the symbol τ for the stress associated with the microstructural constitutive law in equation (20).

The boundary subset $\partial\Omega_t$ has a natural boundary condition $(\sigma = t)$ specified on it. Further, we have $\partial\Omega_u \cap \partial\Omega_t = \varnothing$ and $\overline{\partial\Omega_u \cup \partial\Omega_t} = \overline{\partial\Omega}$.

Introducing the multiscale decomposition at this stage, we apply the following additive split to u and w:

$$u = \underbrace{\bar{u}}_{\text{coarse scale}} + \underbrace{u'}_{\text{fine scale}} \tag{32a}$$

$$w = \underbrace{\bar{w}}_{\text{coarse scale}} + \underbrace{w'}_{\text{fine scale}} \tag{32b}$$

We denote by $\bar{\mathcal{S}}, \bar{\mathcal{V}}$ and $\mathcal{S}' \equiv \mathcal{V}'$, the spaces to which the coarse and fine scale fields belong. Thus,

$$\bar{u} \in \bar{\mathcal{S}}, \quad \bar{w} \in \bar{\mathcal{V}}, \quad u' \in \mathcal{S}', \quad w' \in \mathcal{S}' \tag{33}$$

The fine scale solution is intended to reflect the microstructural behavior.

Clearly, decompositions of the form of equation (32) are fairly general. The following steps make the desired decomposition more precise:

1. It will be required that u' and w' vanish on $\overline{\Omega \backslash \Omega_e}$; that is,

$$u'(x) = w'(x) = 0 \quad \text{on} \quad \overline{\Omega \backslash \Omega_e} \tag{34}$$

Note that $\partial\Omega_e \subset \overline{\Omega \backslash \Omega_e}$.

2. A basis will be defined for $\bar{u}$.

The goal is to develop a model expressed entirely in terms of the coarse scale, which, however, reflects the details of the fine scale. This is achieved by expressing the fine scale, u', in terms of the coarse scale $\bar{u}$, and eliminating u' from the problem statement.

Remark 5. *If* u′ *is to be eliminated from the problem, stability of the formulation requires* $\bar{\mathcal{S}} \cap \mathcal{S}' = \varnothing$. *This is satisfied if the spaces are orthogonal with respect to some inner product.*

Remark 6. *The multiscale decomposition adopted in Hughes*[30] *and Garikipati and Hughes,*[26] *holds for all subdomains* Ω_e *such that* $\overline{\Omega} = \overline{\cup_{e=1}^{n_{el}} \Omega_e}$. *In contrast, a single subdomain* Ω_e *is chosen here, with* $\Omega_e \subset \Omega$, $\Omega_e \neq \Omega$, *and* $\Gamma \in \Omega_e$. *The multiscale decomposition is introduced only over* Ω_e. *The motivation for this choice is that we wish to consider a single discontinuity* Γ. *This does not imply any loss of generality for the developments that follow.*

On substituting equation (32) in the weak form (W), we have

$$\begin{aligned} &\int_{\Omega} (\bar{w}_{,x} + w'_{,x})\sigma\, dV - \int_{\Omega} (\bar{w} + w') f\, dV - \\ &\int_{\partial\Omega_t} (\bar{w} + w') t\, dS = 0 \end{aligned} \tag{35}$$

On using integration by parts and accounting for the surface Γ, we get

$$\begin{aligned} &\int_{\Omega} \bar{w}_{,x}\, \sigma\, dV - \int_{\Omega} \bar{w} f\, dV - \int_{\partial\Omega_t} \bar{w} t\, dS \\ &- \int_{\Omega_e \backslash \Gamma} w' \sigma_{,x}\, dV - \int_{\Omega_e} w' f\, dV - \int_{\partial\Omega_e \cap \partial\Omega_t} w' t\, dS \\ &+ \int_{\partial\Omega_e} w' \sigma\, dS - \int_{\Gamma} w' \sigma^+\, dS + \int_{\Gamma} w' \sigma^-\, dS = 0 \end{aligned} \tag{36}$$

Applying equation (34) and using standard arguments, we arrive at the weak form associated with the fine scale denoted (W'):

$$\begin{aligned} &\int_{\Omega_e \backslash \Gamma} w' \sigma_{,x}\, dV - \int_{\Omega_e} w' f\, dV + \int_{\Gamma} w' \sigma^+ dS \\ &- \int_{\Gamma} w' \sigma^- dS = 0 \end{aligned} \tag{37}$$

and that associated with the coarse scale, denoted $(\bar{W})$:

$$\int_{\Omega} \bar{w}_{,x}\, \sigma\, dV - \int_{\Omega} \bar{w} f\, dV - \int_{\partial\Omega_t} \bar{w} t\, dS = 0 \tag{38}$$

We introduce a second assumption:

Assumption 2. *The space* $\mathcal{S}'$ *contains all nontrivial functions* w' *that vanish on* $\partial\Omega_e \cup (\Omega \backslash \Omega_e)$.

Then, by a standard argument applied to (W'), one arrives at the strong form, denoted (S'), to be solved in Ω_e.

Find $u = \bar{u} + u'$, and σ satisfying (P) in $\Omega_e \backslash \Gamma$ such that

$$\bar{u} \in \bar{S}, \quad u' \in S' \tag{39}$$

$$(S') \qquad \sigma_{,x} + f = 0 \quad \text{in} \quad \Omega_e \backslash \Gamma \tag{40}$$

$$[\![\sigma]\!]_\Gamma = 0 \tag{41}$$

$$u' = 0 \quad \text{on} \quad \partial\Omega_e \tag{42}$$

Remark 7. *The condition cited in Assumption 2 for the space S' is affected by the choice of $\bar{S}$ (i.e., by the choice of basis for $\bar{S}$). In Remark 5, it is pointed out that $\bar{S}$ and S' need to be orthogonal with respect to a suitable inner product for stability of the formulation. This constraint can place restrictions on S', in effect excluding certain functions* W′. *Then the hypothesis made in Assumption 2 may no longer hold and* (W′) *does not imply* (S′). *Choosing $\bar{S}(\Omega_e) = \mathcal{P}^1(\Omega_e)$ (i.e., linear polynomials) circumvents this difficulty, as, then, $\bar{S} \cap S' = \varnothing$ with S' containing all nontrivial functions satisfying equation (34). This choice will be made here.*

$$\bar{S}(\Omega_e) = \mathcal{P}^1(\Omega_e) \tag{43}$$

Equation (41) gives $\sigma|_{\Gamma^-} = \sigma|_{\Gamma^+}$, where

$$\sigma|_{\Gamma^-} := \lim_{x \to \Gamma^-} \sigma, \quad \sigma|_{\Gamma^+} := \lim_{x \to \Gamma^+} \sigma \tag{44}$$

Consistency between the micromechanical model (M), on Γ, and the standard macromechanical description in $\Omega \backslash \Gamma$ will be enforced by requiring

$$\tau = \sigma|_{\Gamma^-} = \sigma|_{\Gamma^+} \tag{45}$$

where τ is the stress corresponding to the microstructural law summarized in (M).
For brevity, $\sigma_\Gamma := \sigma|_{\Gamma^-} = \sigma|_{\Gamma^+}$ will be used in the rest of the development. Thus,

$$\tau = \sigma_\Gamma \tag{46}$$

(with τ governed by (M) on Γ) and equation (40) in $\Omega_e \backslash \Gamma$ must be satisfied simultaneously. Using them, u' will be expressed in terms of $\bar{u}$.

3.2 Solution for the Fine Scale Field

We observe that the following distinct decompositions have been applied to the displacement field in Ω_e: equations (9) and (32a). The two decompositions are related by including the discontinuous component $[\![u]\!] H_\Gamma$ in the fine scale u'. Dispensing with the explicit indication of time dependence, this is written out as follows:

$$u(x) = \underbrace{\bar{u}(x)}_{\text{coarse scale}} + \underbrace{\tilde{u}(x) + [\![u]\!] H_\Gamma(x)}_{\text{fine scale } (u')} \tag{47}$$

The field $\tilde{u}$ introduced above corresponds to the continuous component of the fine scale. Alternatively, we have

$$u(x) = \underbrace{\bar{u}(x) + \tilde{u}(x)}_{\text{continuous displacement } \hat{u}} + [\![u]\!] H_\Gamma(x) \tag{48}$$

The case of interest we will pursue is that of nonlinear, inelastic constitutive relations for σ as a functional of $u_{,x}$ and a vector of internal variables α in $\Omega_e \backslash \Gamma$. Indeed, for a linear, elastic model, strain localization in the sense meant here does not occur (see Section 2 for necessary conditions for the presence of discontinuous displacements). The reader is directed to the paper of Armero and Garikipati,[23] which discusses the necessary conditions for localization of strain into strong discontinuities. In the present situation the nonlinear, inelastic law is written symbolically as follows:

$$\sigma(u_{,x}, \alpha) = \mathcal{N}(u_{,x}, \alpha) \quad \text{in} \quad \Omega_e \backslash \Gamma \tag{49}$$

where α is a vector of internal variables and $\mathcal{N}(\cdot,\cdot)$ is a functional that is nonlinear in $u_{,x}$ and α. In what follows, the explicit dependence on α is suppressed. In general, no analytic solution can be found that expresses u' in terms of $\bar{u}$ through (49), and (40). Following the approach adopted in Garikipati and Hughes,[26] we expand equations (40) and (46), coupled with equation with (20) or (25), to first order about $u_{,x}$ and $[\![u]\!]$. This gives

$$\frac{d}{dx}(\sigma(u_{,x}) + G_t(\Delta\bar{u}_{,x} + \Delta\tilde{u}_{,x})) + f \approx 0 \quad \text{in} \quad \Omega_e^- \cup \Omega_e^+$$

$$\begin{aligned} &\tau([\![u]\!]) + \overline{\mathcal{H}} \Delta[\![u]\!] - \sigma_\Gamma(u_{,x}) - \\ &G_t(\Delta\bar{u}_{,x} + \Delta\tilde{u}_{,x}) \approx 0 \quad \text{on } \Gamma \end{aligned} \tag{50}$$

where G_t is the tangent modulus defined by

$$G_t := \frac{d\sigma}{du_{,x}} \quad \text{in} \quad \Omega_e \backslash \Gamma \tag{51}$$

Here, $u_{,x}$ and $[\![u]\!]$ are not to be regarded as the strain and discontinuous component corresponding to the actual solution, but rather, as zeroth-order approximations. The same holds when $\sigma(u_{,x})$ and $\tau([\![u]\!])$ are evaluated using these quantities. In the iterative solution scheme implied by such a step, $\sigma_\Gamma(u_{,x})$ and $\tau([\![u]\!])$, governed by equation (49) and (M), respectively, are not equal in general; that is, equation (46) is not satisfied.

Remark 8. *Attention is drawn to the strain field, which, from equation (48), can be written as* $u_{,x} = \bar{u}_{,x} + \tilde{u}_{,x} + [u]\delta_\Gamma$. *In* $\Omega_e \backslash \Gamma$, *however,* $\delta_\Gamma = 0$. *Accordingly* $u_{,x} = \bar{u}_{,x} + \tilde{u}_{,x}$ *in* $\Omega_e \backslash \Gamma$. *This property was used in equation (50).*

Now, introducing the operator $\mathcal{L}$, defined as

$$\mathcal{L}(\cdot) := \frac{d}{dx}\left(G_t \frac{d}{dx}(\cdot)\right) \tag{52}$$

and dropping the explicit indication of the arguments, we have the following first-order approximation of the system of equations that must be solved:

$$\mathcal{L}\Delta\tilde{u} = -f - \frac{d\sigma}{dx} - \mathcal{L}\Delta\bar{u} \quad \text{in} \quad \Omega_e \backslash \Gamma \tag{53a}$$

$$\Delta[u] = \frac{1}{\overline{\mathcal{H}}}[\sigma_\Gamma - \tau + G_t(\Delta\bar{u}_{,x} + \Delta\tilde{u}_{,x})] \tag{53b}$$

Using them, $\Delta u'$ will be expressed in terms of $\Delta\bar{u}$. The solution hinges upon the suitable characterization of $\Delta u'$. We have,

$$u'|_{\partial\Omega_e} = 0 \Rightarrow \Delta u'|_{\partial\Omega_e} = 0 \tag{54}$$

When we use the decomposition $u'(x) = \tilde{u}(x) + [u]H_\Gamma(x)$, and recall that $\Omega_e^+ \cup \Gamma$ is the domain in which $H_\Gamma(x) = 1$, this gives

$$\Delta\tilde{u}|_{\partial\Omega_e^-} = 0 \tag{55a}$$

$$\Delta\tilde{u}|_{\partial\Omega_e^+} + \Delta[u] = 0 \tag{55b}$$

Integrating and imposing the boundary conditions of equations (55) on the components of $\Delta u'$ results in expressions for $\Delta\tilde{u}$ and $\Delta[u]$ as linear functionals depending on f, σ, τ, and $\Delta\bar{u}$:

$$\Delta\tilde{u} = \mathcal{F}_1(-f - \sigma_{,y} - \mathcal{L}\Delta\bar{u}) + \mathcal{F}_2(\sigma_\Gamma - \tau + G_t\Delta\bar{u}_{,y}) \tag{56a}$$

$$\Delta[u] = \mathcal{G}_1(-f - \sigma_{,y} - \mathcal{L}\Delta\bar{u}) + \mathcal{G}_2(\sigma_\Gamma - \tau + G_t\Delta\bar{u}_{,y}) \tag{56b}$$

The functionals $\mathcal{F}_1$, $\mathcal{F}_2$, $\mathcal{G}_1$, and $\mathcal{G}_2$ are

$$\begin{aligned}\mathcal{F}_1(g) = &\int_{\Omega_e} K(y,x)G_t^{-1}(y)\int_{\Omega_e} K(z,y)(g(z))dz\,dy \\ &+ \int_{\Omega_e} K(\xi,x)G_t^{-1}(\xi)d\xi \\ &\times\left[\frac{1}{\tilde{G}_0^{-1}}\int_{\Omega_e}\left(\tilde{G}_t^{-1}(y)\int_{\Omega_e} K(z,y)(-g(z))dz\right)dy\right]\end{aligned} \tag{57}$$

$$\begin{aligned}\mathcal{F}_2(g) = &\int_{\Omega_e} K(\xi,x)G_t^{-1}(\xi)d\xi \\ &\times\left[\frac{1}{\tilde{G}_0^{-1}}\int_{\Omega_e}\frac{\delta_\Gamma(y)}{\overline{\mathcal{H}}}(g(y))dy\right]\end{aligned} \tag{58}$$

$$\begin{aligned}\mathcal{G}_1(g) = \frac{1}{\overline{\mathcal{H}}}\Bigg[&\int_{\Omega_e} K(y,\Gamma)(g(y))dy \\ &-\frac{1}{\tilde{G}_0^{-1}}\int_{\Omega_e}\left[\tilde{G}^{-1}(\xi)\int_{\Omega_e}(g(z))K(z,\xi)dz\right]d\xi\Bigg]\end{aligned} \tag{59}$$

$$\mathcal{G}_2(g) = \frac{1}{\overline{\mathcal{H}}}[g(\Gamma)] - \frac{1}{\tilde{G}_0^{-1}}\int_{\Omega_e}\delta_\Gamma(\xi)(g(\xi))d\xi \tag{60}$$

The terms $K(x, y)$, $\tilde{G}^{-1}$ and $\tilde{G}_0^{-1}$ are given by

$$\begin{aligned}K(x,y) &= 1 - H_y(x) \\ \tilde{G}^{-1}(y) &= G_t^{-1}(y) + \frac{\delta_\Gamma(y)}{\overline{\mathcal{H}}} \\ \tilde{G}_0^{-1} &= \int_{\Omega_e}\tilde{G}_t^{-1}(y)dy\end{aligned} \tag{61}$$

In equations (58), (60), and (61), δ_Γ is the Dirac delta function located at Γ.

It now remains to eliminate the fine scale components from $(\overline{W})$, the weak form associated with the coarse scale. This will result in a weak form functionally free of the fine scale, yet accounting for its effect.

3.3 The Weak Form for $\Delta\bar{u}$

Distributional considerations lead to the conclusion that σ must be a regular distribution in Ω. Briefly, this result is arrived at as follows. Under the assumption of strong discontinuities in the displacement field, the plastic dissipation, denoted $\mathcal{D}_\Omega$, is expressed as (see Simo et al.[20] for details):

$$\mathcal{D}_\Omega = \int_\Omega \sigma\dot{\varepsilon}^p dV + \frac{1}{2}\int_\Omega\left(q\gamma + \dot{q}\int_0^t \gamma(s)ds\right)dV \tag{62}$$

Recalling the flow rule from equation (2), this gives

$$\mathcal{D}_\Omega = \int_\Omega \sigma\gamma\partial_\tau\phi dV + \frac{1}{2}\int_\Omega\left(q\gamma + \dot{q}\int_0^t \gamma ds\right)dV \tag{63}$$

With γ being a singular distributional quantity [i.e., as in equation (14)] and q and $\dot{q}$ being regular (see Section 2.4), it follows that for the plastic dissipation to be physically meaningful and mathematically well defined, the stress itself must be regular.

Now, recalling the weak form $(\overline{W})$, and observing that the integrand of $\int_{\Omega} \overline{w}_{,x}\,\sigma dV$ is a regular distribution, the integral is equal to $\int_{\Omega\backslash\Gamma} \overline{w}_{,x}\,\sigma dV$ (see Kolmogorov and Fomin [31] for details)

$$\int_{\Omega\backslash\Gamma} \overline{w}_{,x}\sigma dV = \int_{\Omega} f\,dV + \int_{\partial\Omega} \overline{w}\,t\,dS \tag{64}$$

The incremental fine scale field is introduced by writing out the first-order approximation to σ in equation (53a):

$$\begin{aligned} &\int_{\Omega\backslash\Gamma} \overline{w}_{,x}(\sigma + G_t(\Delta\overline{u}_{,x} + \Delta\widetilde{u}_{,x})dV = \\ &\int_{\Omega} \overline{w} f\,dV + \int_{\partial\Omega} \overline{w}\,t\,dS \end{aligned} \tag{65}$$

Integrating by parts, we can write

$$\begin{aligned} &\int_{\Omega\backslash\Gamma} \overline{w}_{,x} G_t \Delta\overline{u}_{,x}\,dV - \int_{\Omega_e\backslash\Gamma} (G_t\overline{w}_{,x})_{,x}\,\Delta\widetilde{u}\,dV + \\ &\int_{\partial\Omega_e^+} \overline{w}_{,x}\,G_t\Delta\widetilde{u}\,dS - \underbrace{\int_{\partial\Omega_e^-} \overline{w}_{,x}\,G_t\Delta\widetilde{u}\,dS}_{=0} = \\ &\int_{\Omega} \overline{w} f\,dV - \int_{\Omega\backslash\Gamma} \overline{w}_{,x}\,\sigma dV + \int_{\partial\Omega_t} \overline{w}\,t\,dS \end{aligned} \tag{66}$$

In the relation above the boundary condition on $\Delta\widetilde{u}$ at $\partial\Omega_e^-$ is applied to eliminate the fourth term on the left-hand side.

Remark 9. *Equation (64) exploits a result according to which Lebesgue integrals involving regular distributional integrands remain unchanged when a subset of the domain of integration with zero measure is excluded when evaluating the integral. This step is crucial, since it allows* σ *to be expanded over* $\Omega\backslash\Gamma$. *As a consequence, terms involving* $d(H_\Gamma[\![u]\!])/dx = \delta_\Gamma(x)[\![u]\!]$ *are absent in the first-order approximation and the continuous component of* $\Delta u'$*; that is,* $\Delta\widetilde{u}$ *alone makes an appearance.*

The bilinear forms

$$a(\overline{w},\Delta\overline{u})_{\Omega} = \int_{\Omega} \overline{w}_{,x}\,G_t\Delta\overline{u}_{,x}\,dV \quad \text{(symmetric)} \tag{67}$$

$$b(\overline{w},\Delta\widetilde{u})_{\partial\Omega} = \int_{\partial\Omega} \overline{w}_{,x}\,G_t\Delta\widetilde{u}\,dS \quad \text{(unsymmetric)} \tag{68}$$

the operator $\mathcal{L}^*$ (adjoint of $\mathcal{L}$), and the inner product $(\cdot,\cdot)_{\Omega}$ are introduced. Now, the weak form can be written as follows:

$$\begin{aligned} &a(\overline{w},\Delta\overline{u})_{\Omega} - (\mathcal{L}^*\overline{w},\Delta\widetilde{u})_{\Omega_e} + b(\overline{w},\Delta\widetilde{u})_{\partial\Omega_e^+} \\ &\quad = (\overline{w},f)_{\Omega} - (\overline{w}_{,x},\sigma)_{\Omega\backslash\Gamma} + (\overline{w},t)_{\partial\Omega} \end{aligned} \tag{69}$$

Substituting for $\Delta\widetilde{u}$ from equation (56a), the weak form that needs to be solved for $\Delta\overline{u}$ is

$$\begin{aligned} &a(\overline{w},\Delta\overline{u}) - (\mathcal{L}^*\overline{w},\mathcal{F}_1(-\mathcal{L}\Delta\overline{u}))_{\Omega_e} + b(\overline{w},\mathcal{F}_1(-\mathcal{L}\Delta\overline{u}))_{\partial\Omega_e^+} \\ &\quad -(\mathcal{L}^*\overline{w},\mathcal{F}_2(G_t\Delta\overline{u}))_{\Omega_e} + b(\overline{w},\mathcal{F}_2(G_t\Delta\overline{u}))_{\partial\Omega_e^+} \\ (\overline{\mathcal{W}}) \quad &\quad = (\overline{w},f)_{\Omega} + (\overline{w},t)_{\partial\Omega_t} - (\overline{w}_{,x},\sigma)_{\Omega\backslash\Gamma} \\ &\quad +(\mathcal{L}^*\overline{w},\mathcal{F}_1(-f-\sigma_{,y}))_{\Omega_e} - b(\overline{w},\mathcal{F}_1(-f-\sigma_{,y}))_{\partial\Omega_e^+} \\ &\quad +(\mathcal{L}^*\overline{w},\mathcal{F}_2(\sigma_\Gamma-\tau))_{\Omega_e} - b(\overline{w},\mathcal{F}_2(\sigma_\Gamma-\tau))_{\partial\Omega_e^+} \end{aligned} \tag{70}$$

This is the weak form of the multiscale method, denoted $(\overline{\mathcal{W}})$, for the microstructural model under consideration. While $(\overline{\mathcal{W}})$ is expressed solely in terms of the incremental coarse scale field, it accounts for the incremental fine scale field. This weak form is the basis for computations.

Remark 10. *On solving for* $\Delta\overline{u}$ *(e.g., using the finite element method),* $\Delta u'$ *can be recovered via equations (56) to (60). These incremental fields are added to the approximate total solution* u, *to arrive at a corrected total solution. In general, on evaluating* σ *and* τ *from the corrected total solution, one will find that equations (40) and (45) have not been satisfied. An iterative procedure such as the Newton–Raphson method must be applied to solve the nonlinear problem. Note that crucial elements of the present multiscale formulation such as the incremental fields, the tangent modulus, and the Newton–Raphson method are typical of algorithmic implementations of nonlinear constitutive models. Accordingly, the entire development can be viewed as being applied to an algorithmic version of the problem.*

Remark 11. *Since* $\Delta u' = 0$ *on* $\partial\Omega_e$ *in equation (56), it follows that* $u' = 0$ *and therefore* $\overline{u}$ *itself must be exact on* $\partial\Omega_e$.

Remark 12. *Note that in the weak form* $(\overline{W})$, *only the continuous component of* $\Delta u'$ *(i.e.,* $\Delta\widetilde{u}$ *) needs to*

be substituted. However, $\Delta\tilde{u}$ itself is dependent on $\Delta[\![u]\!]$ through equation (55). The boundary terms arising from $(\overline{w}_{,x}, G_t\Delta\tilde{u})$ introduce this dependence in $(\overline{W})$. These terms constitute crucial differences in the weak form of the multiscale method for this problem in comparison with the corresponding weak form in Garikipati and Hughes.[26]

Remark 13. *The development leading to equation (70) has been carried out under the assumption that there is a single discontinuity Γ, which lies in element Ω_e (see Remark 6). The extension to multiple discontinuities is straightforward. It merely requires that the integrals presently evaluated on Ω_e and $\partial\Omega_e^+$ be evaluated for all elements Ω_e that contain a discontinuity and their boundaries $\partial\Omega_e^+$, respectively.*

The development described above does not take into account the possibility that the stress on Γ (i.e., τ) may unload. The multiscale formulation of the problem for this case is described in Section 3.4.

3.4 The Multiscale Formulation for Unloading on Γ

For the strong discontinuities model, unloading takes place elastically. The discontinuous component $[\![u]\!]$ can be interpreted as an internal variable that models the shrinking of the admissible domain (in one-dimensional stress space) for the stress on the discontinuity [see equations (24)–(27)]. Recalling that the development of the strong discontinuities model is based on plastic flow in a softening continuum [see equations (1)–(6)] and that the discontinuous displacement $[\![u]\!]$ is identified with the (singular) plastic multiplier through equation (15), we can see that for elastic unloading, $[\![u]\!]$ does not evolve. To arrive at a formulation that recovers this property, the algorithmic implementation of the strong discontinuities model is chosen as the point of departure (see Remark 10 above). The algorithmic model is described in Garikipati[32] (p.139). It is summarized here.

Let the time interval $[0,T]$ be discretized into N subintervals via time instants $\{t_0, t_1, \ldots, t_n, \ldots, t_N\}$, with $t_0 = 0$ and $t_N = T$. Using time as a parameter, let the load be applied in discrete increments (load or displacement control). Consider an incremental load step between t_n and t_{n+1}. An iterative process is to be applied to the nonlinear constitutive relations to find the solution at t_{n+1}. Let $(\cdot)_n$ denote the algorithmic value of a quantity of interest at time t_n. These quantities are converged values. The algorithmic quantities at the $(i+1)$th iteration of the $(n+1)$th time step are denoted $(\cdot)_{n+1}^{i+1}$. The algorithm for this iteration appears in the accompanying box.

```
Iteration i+1
1. On Γ, ε_{n+1}^{TR,(i+i)} := ū_x, [u]_{n+1}^{TR,(i+1)} := [u]_n
   ε_{n+1}^{p,TR} := ε_n^p |_{Ω_e\Γ}
   Given [u]_{n=1}^{(i+1)}
2. τ_{n+1}^{TR,(i+1)} := G(ε_{n+1}^{TR,(i+i)} − ε_{n+1}^p)
3. ψ_{n+1}^{TR,(i+1)} := |τ_{n+1}^{TR,(i+1)}| − (τ_Y + H̄|[u]_{n+1}^{TR,(i+1)}|)
4. IF (ψ_{n+1}^{TR,(i+1)} < 0) THEN (elastic unloading)
      [u]_{n+1}^{(i+1)} := [u]_n, τ_{n+1}^{(i+1)} := τ_{n+1}^{TR,(i+1)}
      EXIT
ELSE (loading)
      |τ_{n+1}^{(i+1)}| := τ_Y + H̄|[u]_{n+1}^{TR,(i+1)}|
      EXIT
ENDIF
```

In the boxed algorithm, G is the elastic shear modulus. If $[\![u]\!]$ does not evolve during the current iteration, we have $\Delta u = \Delta\overline{u} + \Delta\tilde{u}$. Then, recalling equation (45), and dispensing with the subscripts denoting the current instant in the solution, we find that the equation to be solved on Γ is

$$\sigma_\Gamma - \tau = 0$$

and its first-order approximation is

$$\sigma_\Gamma - \tau + G(\Delta\overline{u}_{,x} + \Delta\tilde{u}_{,x}) - G\Delta\overline{u}_{,x} \tag{71}$$

where $\Delta u_{,x} = \Delta\overline{u}_{,x} + \Delta\tilde{u}_{,x}$ in $\Omega_e\backslash\Gamma$ has been used in the first-order approximation of σ_Γ and elastic unloading in $\Omega_e\backslash\Gamma$ has been assumed. As before, σ_Γ and τ in equation (71) are evaluated on the basis of fields that do not necessarily ensure satisfaction of equations (40) and (45). The nonlinear problem is solved by applying the Newton–Raphson method to this first-order approximation. The relation above gives

$$\Delta\tilde{u}_{,x}\big|_\Gamma = -\left(\frac{\sigma_\Gamma - \tau}{G}\right) \tag{72}$$

From equations (53a) and (52), we write

$$\mathcal{L}\Delta\tilde{u} = -f - \frac{d\sigma}{dx} - \mathcal{L}\Delta\overline{u} \tag{73}$$

where, since elastic unloading prevails, $\mathcal{L}(\cdot) = d/dx(G[d(\cdot)/dx])$. Using the boundary condition of equation (55a), we can solve equations (72) and (73) simultaneously to give

$$\Delta\tilde{u} = \mathcal{J}_1\left(-f - \frac{d\sigma}{dz} - \mathcal{L}\Delta\bar{u}\right) + \mathcal{J}_2(-(\sigma_\Gamma - \tau)) \quad (74)$$

The functionals $\mathcal{J}_1$ and $\mathcal{J}_2$ are defined as follows:

$$\begin{aligned}\mathcal{J}_1(g) := &\int_{\Omega_e} K(y,x)G^{-1}(y)\left[\int_{\Omega_e} K(z,y)g(z)dz\right]dy \\ &- \int_{\Omega_e} K(y,x)G^{-1}(y)\left[\int_{\Omega_e} K(z,\Gamma)g(z)dz\right]dy\end{aligned} \quad (75)$$

and

$$\mathcal{J}_2(g) := g\int_{\Omega_e} K(y,x)G^{-1}(y)dy \quad (76)$$

As in the case of loading on Γ, the final step involves elimination of the field $\Delta\tilde{u}$ from the weak form. Following the sequence of equations (65) to (69), we have

$$\begin{aligned}a(\bar{w},\Delta\bar{u})_\Omega - (\mathcal{L}^*\bar{w},\Delta\tilde{u})_{\Omega_e} + b(\bar{w},\Delta\tilde{u})_{\partial\Omega_e^+} \\ = (\bar{w},f)_\Omega + (\bar{w},t)_{\partial\Omega_t} - (\bar{w}_{,x},\sigma)_{\Omega\setminus\Gamma}\end{aligned} \quad (77)$$

Substituting for $\Delta\tilde{u}$ as a functional given by equation (74), we arrive at the following expression for the weak form of the multiscale model for unloading:

$$\begin{aligned}&a(\bar{w},\Delta\bar{u})_\Omega - (\mathcal{L}^*\bar{w},\mathcal{J}_1(-\mathcal{L}\Delta\bar{u}))_{\Omega_e} + b(\bar{w},\mathcal{J}_1(-\mathcal{L}\Delta\bar{u}))_{\partial\Omega_e^+} \\ &= (\bar{w},f)_\Omega + (\bar{w},t)_{\partial\Omega_t} - (\bar{w}_{,x},\sigma)_{\Omega\setminus\Gamma} \\ (\overline{W}),\quad &+ (\mathcal{L}^*\bar{w},\mathcal{J}_1(-f-\sigma_{,y}))_{\Omega_e} \\ &- b(\bar{w},\mathcal{J}_1(-f-\sigma_{,x}))_{\partial\Omega_e^+} \\ &+ (\mathcal{L}^*\bar{w},\mathcal{J}_2(-\sigma_\Gamma+\tau))_{\Omega_e} \\ &- b(\bar{w},\mathcal{J}_2(-\sigma_\Gamma+\tau))_{\partial\Omega_e^+}\end{aligned} \quad (78)$$

With this, the multiscale formulation for the microstructural model of strong discontinuities is complete. Its finite element implementation is presented next.

4 FINITE ELEMENT FORMULATION

This section discusses the computational formulation based on the weak form $(\overline{W})$, which was derived in Section 3. Mainly, this involves the choice of $\bar{u}$ and evaluation of certain terms in the weak form.

4.1 Choice of $\bar{u}$

Recall that the weak form to be used as the basis for computations [i.e., $(\overline{W})$] is now expressed entirely in terms of $\Delta\bar{u}$. The association of $\bar{u}$ with a "coarse scale" field suggests that all that is needed is for $\bar{u}$ (and therefore $\Delta\bar{u}$) to be an approximate solution to the problem (W). Accordingly, in a computational setting, using (for instance) the finite element method, $\bar{u}$ is taken to be the finite element interpolate, u^h. The fine scale field u' is the "correction" that gives the total solution u:

$$\bar{u} = u^h \quad \text{and} \quad u' = u - u^h \quad (79)$$

where, in keeping with convention, the superscript h is used to denote approximate quantities. In a finite element context, the subdomain Ω_e is now seen to be an element. In light of Remark 11, u^h is nodally exact.

Furthermore, in keeping with the comments in Remark 7, $\bar{u}$ is linearly interpolated within Ω_e:

$$\bar{u}_e(x) = \sum_{A=1}^{2} N_e^A(x)\bar{d}^A \quad (80)$$

where, $N_e^A(x)$ are linear interpolations and $\bar{d}^A$ are nodal values.

4.2 Discrete Formulation of $\overline{W}$

The weak form $(\overline{W})$ contains terms of the form $\mathcal{L}(\cdot)$, $\mathcal{L}^*(\cdot)$ and $d\sigma/dx$. The operator $\mathcal{L}$ and its adjoint $\mathcal{L}^*$ here take the form

$$\begin{aligned}\mathcal{L}(\cdot),\quad \mathcal{L}^*(\cdot) &:= \frac{d}{dx}\left(G_t\frac{d(\cdot)}{dx}\right) \\ &= \frac{d}{dx}G_t\frac{d(\cdot)}{dx} + G_t\frac{d^2(\cdot)}{dx^2}\end{aligned} \quad (81)$$

The discrete formulation thus involves the evaluation of terms of the form dG_t/dx and, additionally, $d\sigma/dx$, which are nonstandard in finite element formulations. This is accomplished as follows:

1. Given quadrature points z_l, $l \in \{1,\ldots,l_{\text{int}}\}$, and associated weights w_l (Figure 3) in a typical element $[x_e, x_{e+1}]$ of length h, define "interface points" y_k, $k \in \{1,\ldots,l_{\text{int}}-1\}$ internal to the element.

$$y_k = x_e + h\left(\frac{\sum_{i=1}^{k} w_i}{\sum_{i=1}^{l_{\text{int}}} w_i}\right) \quad (82)$$

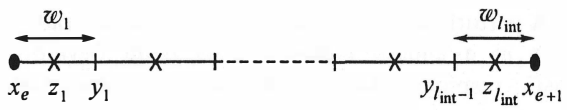

Figure 3. Quadrature points, interface points, and weights

2. Over each of the subdomains in $\{(x_e, y_1), \ldots, (y_{l_{\text{int}}-1}, x_{e+1})\}$, the quantity $(\cdot)$ (G_t or σ) is taken to be a constant. Thus, in a distributional sense,

$$\frac{d}{dx}(\cdot) = \sum_{k=1}^{l_{\text{int}}-1}\left((\cdot)\big|_{z_{k+1}} - (\cdot)\big|_{z_k}\right)\delta_{y_k}(x) \tag{83}$$

with δ_{y_k} being the Dirac delta distribution located at y_k.

4.3 Iterative Solution Procedure

The weak form of the multiscale method, $(\overline{\mathcal{W}})$, is to be solved for $\Delta\overline{u}$, from which the continuous and discontinuous components of $\Delta u'$ can be recovered using equations (56) to (60) [alternatively, equation (74), with (75) and (76) for unloading on Γ]. Following the comments in Remark 10, the approach adopted consists of solving the model of Section 3 by an iterative procedure of the Newton–Raphson type. This ensures solution of the fully nonlinear problem. The procedure is summarized below.

Starting with the weak form of the multiscale formulation, $(\overline{\mathcal{W}})$, letting the coarse scale weighting function $\overline{w}$ be the linear interpolate of nodal values $\overline{c}^A$ (as was done for $\overline{u}$), we have

$$\overline{w} = \sum_{A=1}^{2} N_e^A(x)\overline{c}^A \tag{84}$$

The discrete version of $(\overline{\mathcal{W}})$, written as an assembly over all elements, is

$$\mathop{\mathbf{A}}_{e=1}^{n_{\text{el}}}\left(\overline{\mathbf{c}}_e^T\mathbf{K}_e\Delta\overline{\mathbf{d}}_e\right) = \mathop{\mathbf{A}}_{e=1}^{n_{\text{el}}}\left(\overline{\mathbf{c}}_e^T\mathbf{F}_e\right) \tag{85}$$

and the assembled system of equations to be solved is

$$\overline{\mathbf{c}}^T\mathbf{K}\Delta\overline{\mathbf{d}} = \overline{\mathbf{c}}^T\mathbf{F} \tag{86}$$

In the relation above, $\overline{\mathbf{d}}$ and $\overline{\mathbf{c}}$ are, respectively, the nodal values of the solution and the weighting function, and $\mathbf{K}$ and $\mathbf{F}$ are, respectively, the global, assembled stiffness matrix and the residual vector,

$$\mathbf{K} = \mathop{\mathbf{A}}_{e=1}^{n_{\text{el}}}\mathbf{K}_e \quad \mathbf{F} = \mathop{\mathbf{A}}_{e=1}^{n_{\text{el}}}\mathbf{F}_e \tag{87}$$

The local computation of stress and updating of coarse and fine scale fields is summarized in the box for the $(i+1)$th global iteration.

GLOBAL `iteration` $i+1$

Given $\left\{u^{(i)}, \overline{u}^{(i)}, u'^{(i)}, \sigma^{(i)}, G_t^{(i)}\right\}$

1. $\Delta\overline{\mathbf{d}}^{(i)} = \mathbf{K}^{(i)-1}\mathbf{F}^{(i)}$

LOCAL (element e)

2. $\Delta\overline{u}^{(i)}(x) = \sum_{A=1}^{n_{\text{nodes}}} N_e^A(x)\Delta\overline{d}_e^{A(i)}$
3. Loading on Γ:

$$\Delta\widetilde{u}^{(i)} = \mathcal{F}_1\left(-f - \frac{d\sigma^{(i)}}{dz} - \mathcal{L}\Delta\overline{u}^{(i)}\right) + \mathcal{F}_2\left(\sigma_\Gamma^{(i)} - \tau^{(i)} + G_t\frac{d\Delta\overline{u}^{(i)}}{dz}\right)$$

$$\Delta[\![u]\!]^{(i)} = \mathcal{G}_1\left(-f - \frac{d\sigma^{(i)}}{dz} - \mathcal{L}\Delta\overline{u}^{(i)}\right) + \mathcal{G}_2\left(\sigma_\Gamma^{(i)} - \tau^{(i)} + G_t\frac{d\Delta\overline{u}^{(i)}}{dz}\right)$$

Unloading on Γ

$$\Delta\widetilde{u}^{(i)} = \mathcal{J}_1\left(-f - \frac{d\sigma^{(i)}}{dz} - \mathcal{L}\Delta\overline{u}\right) + \mathcal{J}_2(-(\sigma_\Gamma^{(i)} - \tau^{(i)}))$$

$$\Delta[\![u]\!]^{(i)} = 0$$

4. $\Delta u'^{(i)} = \Delta\widetilde{u}^{(i)} + \Delta[\![u]\!]^{(i)}H_\Gamma(x)$
5. $\Delta u^{(i+1)}(x) = \overline{u}^{(i)}(x) + \Delta\overline{u}^{(i)}(x) + u'^{(i)}(x) + \Delta u'^{(i)}(x)$
6. $\sigma^{(i+1)} = \mathcal{N}(u_{,x}^{(i+1)}, \alpha^{(i+1)})$ in $\Omega\backslash\Gamma$
7. FORM $\mathbf{K}_e^{(i+1)}$ & $\mathbf{F}_e^{(i+1)}$

GLOBAL

8. FORM $\mathbf{F}^{(i+1)} = \mathbf{A}_{e=1}^{n_{\text{el}}}\mathbf{F}_e^{(i+1)}$
9. IF $\left(\left\|\mathbf{F}^{(i+1)}\right\| \le \text{TOL}\right)$ THEN
   EXIT
   ELSE
   $i \to i+1$, GOTO 1
   ENDIF

5 NUMERICAL SIMULATIONS

The multiscale model for strong discontinuities is applied to be numerical solution of strain-softening problems. The underlying model that holds in $\Omega\backslash\Gamma$ is

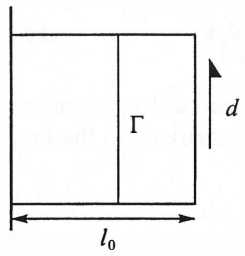

Figure 4. The boundary value problem.

the rate-independent plasticity model described in equations (1) to (6). It is applied to numerical simulations with perfect plasticity in $\Omega \backslash \Gamma$; that is, $\mathcal{H} = 0$. The particular boundary value problem chosen appears in Figure 4. Material properties and problem dimensions appear in Table 1.

Table 1. Material Properties and Problem Dimensions for the Numerical Example

Property	Value
G	1.0
$\mathcal{H}$	0
τ_Y	1.0
l_0	10.0
$\overline{\mathcal{H}}$	−0.001

A perturbation is introduced in τ_Y at a quadrature point in a chosen element. This point develops plastic response, which is the necessary condition for appearance of the discontinuous solutions (see Remark 4). No length scale is associated with the perturbation. The strains localize on the surface Γ and the displacement field develops a discontinuity, $[\![u]\!]H_\Gamma$ (compare with the numerical example in Simo et al.[20]). The first set of plots show the development of fine and coarse fields. Observe the discontinuity in the solution that is carried in the fine scale field. The total field is exact.

The formulation of strain localization in terms of strong discontinuities leads to solutions independent of mesh size (see Armero and Garikipati[23]). This property is inherited when this formulation is cast into the multiscale method. Figure 5 demonstrates this by means of two meshes for the present problem, one having twice as many elements as the other. Observe that the load–displacement curves for the two discretizations are indistinguishable.

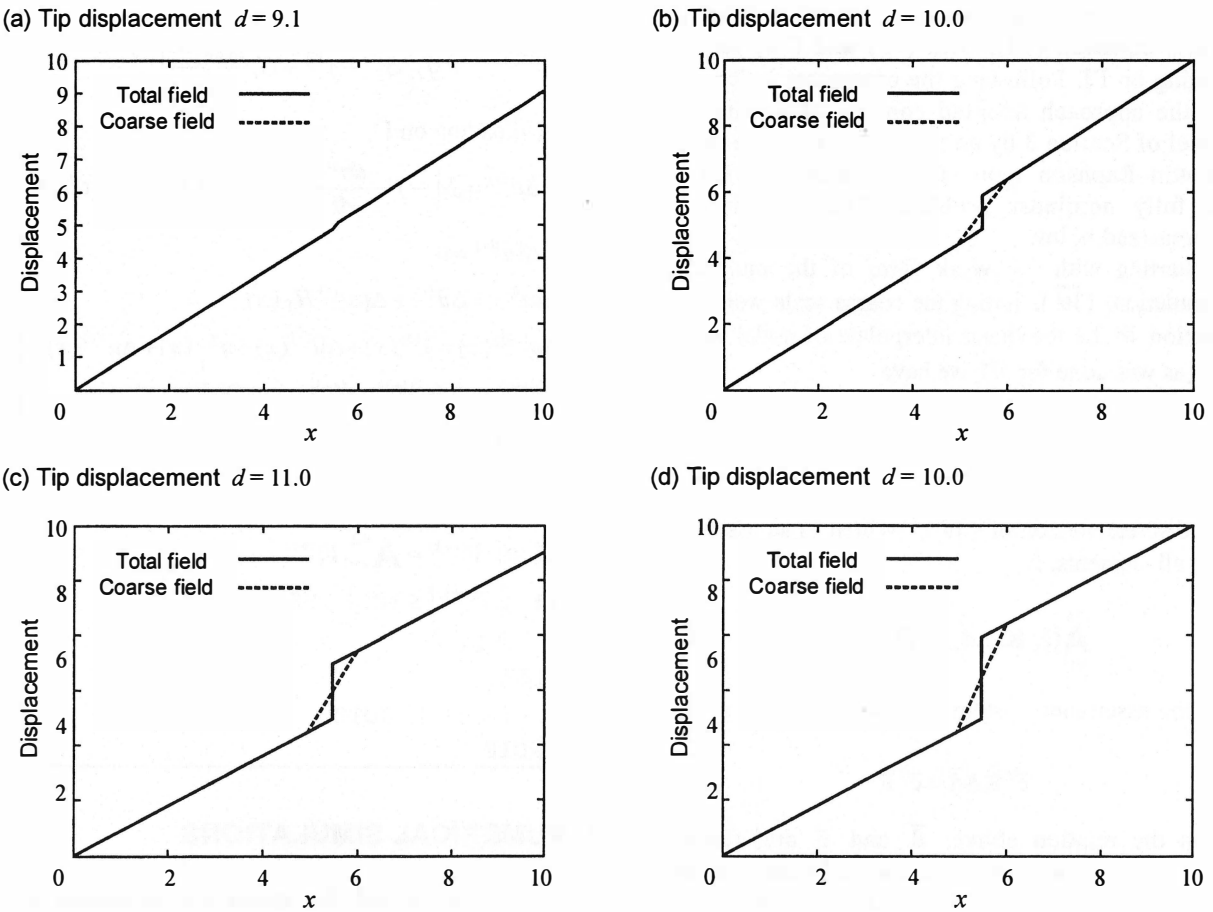

Figure 5. Discontinuous solutions and multiscale fields for a strain-softening problem.

6 CLOSURE

The developments presented in this work extend the framework of the multiscale method for strain localization problems to the case of strong discontinuities. The analysis of standard inelastic constitutive models in the context of strong discontinuities results in an evolution equation for the discontinuous component of the displacement. The approach taken here is to view this evolution equation as the constitutive law of a microstructural model. The framework of multiscale analysis is used to embed this constitutive law in the standard, macromechanical framework.

Making the extension to strong discontinuities provides a degree of completeness to the project of studying strain localization problems in a framework of multiscale solutions. Probably more importantly, the ideas developed here should be viewed as a first step toward extending multiscale analysis to cover related areas in solid mechanics. One possible application is the bridging of length scales — from atomistic to continuum descriptions of behavior of solids — in the treatment of material failure. The application of the multiscale method as a broad framework for analysis also requires an extension to multiple dimensions (see Garikipati and Hughes[33]) and finite strain kinematics.

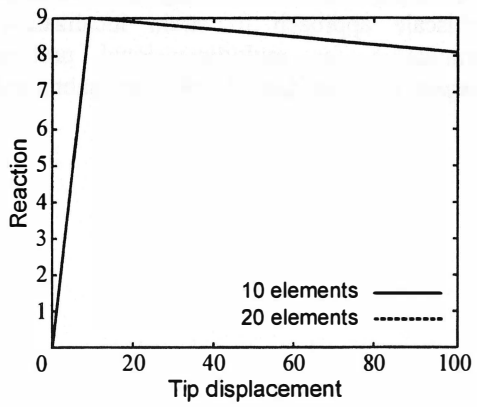

Figure 6. Invariance of load-displacement curves to element size.

ACKNOWLEDGMENT

Funds for this research were provided by the Office of Naval Research under grant N00014-96-1-0109 to Stanford University. This support is greatly appreciated.

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