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An extended multiscale principle of virtual velocities approach for evolving microstructure

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Abstract

A hierarchical multiscale approach is presented for modeling microstructure evolution in heterogeneous materials. Preservation of momentum across each scale transition is incorporated through the application of the principle of virtual velocities at the fine scale giving rise to the appropriate continuum momentum balance equations at the coarse scale. In addition to satisfying momentum balance and invariance of momentum among scales, invariance of elastic free energy, stored free energy, and dissipation between two scales of observation is regarded as crucial to the physics of each scale transition. The preservation of this energy partitioning scheme is obtained through construction of constitutive relations within the framework of internal state variable theory. Internal state variables that are directly computed from the fine scale response are introduced to augment the state equations and describe the inelastic energy storage and dissipation within the fine scale. By virtue of a second gradient kinematic decomposition, the framework naturally gives rise to couple stresses.

Keywords: multiscale; principle of virtual velocities; dissipation; scale invariance; microstructure evolution; second gradient; strain gradient

1. Introduction

Multiscale modeling seeks to address the response of heterogeneous materials at varying levels of resolution and at varying scales of physics. Presented here is a general set of principles that establish a framework for ensuring the physical consistency of models of irreversible microstructure evolution at multiple scales. This particular framework is being developed to transition between scales of material response that are each amenable to a continuum description; however, the principles are more general and could be applied to atomistic to continuum scale linking, for example, cf. [1]. We focus on the sequential hierarchical approach, but the same principles can hold value for concurrent approaches, in which the solutions for all scales of interest are generated simultaneously.

In addition to the satisfaction of classical continuum laws at each scale, the issues central to this framework are maintaining kinematic consistency and the invariance of mass, linear and angular momentum, and energy with

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respect to the scale at which a given set of mass particles are observed. Furthermore, we assert that in addition to scale invariance of the total energy, the partition of total energy into recoverable, stored, and dissipated energy shall also be invariant with respect to the scale at which a given set of mass particles are observed.

2. Hierarchy of Scales

A general hierarchy of N scales is depicted in Figure 1. Every material point, identified by the vector position $\mathbf{x}_o$, in the scale 0 continuum represents the behavior of a neighborhood of material response, ${}^x\Omega_o^1$, at scale 1 (finer than scale 0). This neighborhood of material points at scale 1 is defined by the referential statistical volume element (rSVE), which is not necessarily a referential *representative* volume element (rRVE) in the rigorous sense. The local constitutive behavior of each material point, identified by the vector position $\mathbf{y}_o$ in the scale 1 coordinate system, within the rSVE domain, ${}^x\Omega_o^1$, at scale 1 is defined by a free energy function, mechanical strain, temperature, a set of internal state variables, and corresponding evolution equations that are derived as necessary from computational simulations of the rSVE at scale 2. In general, the transition to a coarser scale, *k*, is performed by solving the initial boundary value problem for an rSVE of material points at scale *k+1*, as shown in Figure 2. In this process, new internal state variables are introduced to represent kinematic degrees of freedom at scale *k+1*. Simultaneously, those internal state variables (ISVs) associated with the kinematic degrees of freedom at scale *k+2* are *released*. Therefore, ISVs from scale *k+2* and finer are only present at scales *k* and higher due to their implicit mapping into the newly introduced ISVs at scale *k*. In other words, as the scale of observation increases, the number of degrees of freedom used to quantify kinematics of the finest scales decreases. Conceptually, this suggests that one cannot ascertain details of the fine scale response while observing from the coarse scale. The physical manifestation is that, through the hierarchy of scale transitions, dissipation and locally stored energy are smeared from scale to scale. Practically, the result is that each significant process at each significant scale will require detailed study to develop appropriate scale specific constitutive relations. It is inappropriate, in general, to simply use the volume average of finer scale constitutive relations to model the response of coarser scales if we insist on the aforementioned invariance requirements, as will be shown.

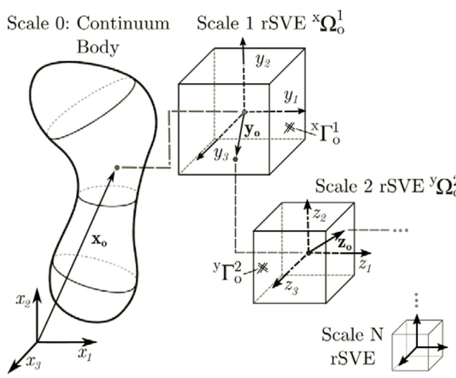

Figure 1. General N-scale hierarchy

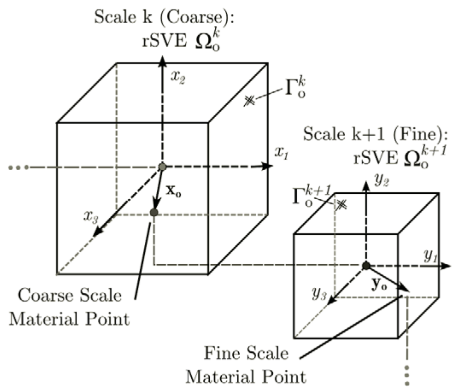

Figure 2. Depiction of a single transition in scale.

3. Multiscale Framework

3.1. Kinematic Consistency

Deformation of the rSVE at two scales of observation must be kinematically consistent. Kinematic consistency is realized by requiring that the description of deformation be the same at each scale with the exception of a fluctuation field whose mean value vanishes over certain length scales. The general idea is that the smooth long-wavelength deformation is the same at coarse and fine scales, while fine scale heterogeneity is accommodated by fluctuations over wavelengths that cannot be directly resolved at the coarse scale. Fine scale fluctuations in deformation should have zero projection onto coarse scale kinematic variables. Furthermore, the kinematic decomposition of the fine scale deformation must be uniquely associated with coarse scale kinematic variables. The most direct way to accommodate this demand is to ensure orthogonality of independent contributions to the fine-scale deformation. For example, using a second order Taylor series expansion of the fine scale deformation field, i.e.,

$$\underbrace{\mathbf{y}(\mathbf{x}_o,\mathbf{y}_o)}_{\text{fine scale}} = \underbrace{\mathbf{C}(\mathbf{x}_o)+\mathbf{F}(\mathbf{x}_o)\cdot\mathbf{y}_o+\tfrac{1}{2}\mathbf{G}(\mathbf{x}_o):\mathbf{y}_o\otimes\mathbf{y}_o}_{\text{coarse scale expansion}} + \underbrace{\mathbf{h}(\mathbf{y}_o)}_{\substack{\text{fine scale}\\ \text{fluctuation}}} \tag{1}$$

the fine scale deformation gradient is decomposed into $\mathbf{f}=\mathbf{f}^1+\mathbf{f}^2+\mathbf{f}^3$ where $\mathbf{f}^1=\mathbf{F}$, $\mathbf{f}^2=\mathbf{G}\cdot\mathbf{y}_o$, and $\mathbf{f}^3=\mathbf{h}\bar{\nabla}$ and kinematic consistency between the coarse and fine scales is achieved by requiring $\int \mathbf{f}^i\cdot\mathbf{f}^j d\Omega_o=\mathbf{0}$ for $i\neq j$.

The particular kinematic decomposition (1) selected here implies a micromorphic continuum theory [2] and, for the case where $\mathbf{F}=\mathbf{x}\bar{\nabla}$ is the coarse scale deformation gradient and $\mathbf{G}=\mathbf{F}\bar{\nabla}$ is the coarse scale gradient of the deformation gradient, results in a second-gradient continua at the coarse scale [3, 4]. The second gradient, $\mathbf{G}$, kinematically related to strain gradients and curvature [5], is employed in other multiscale modeling approaches [6-9] .

3.2. Scale Invariance of Linear Momentum

It is a fundamental requirement of continuum theories at all scales that momentum must be balanced, giving rise to continuum equations of motion. At any particular scale, computational methods (e.g. finite element) are employed to solve the initial boundary value problem in accordance with linear momentum balance. Linear momentum is a fundamental quantity that should be invariant with respect to the scale of observation. In practice, this principle guides the derivation of coarse scale stress terms conjugate with the coarse scale description of the fine scale deformation and consistent with the distribution of fine scale stresses and inertia via the principle of virtual velocities (PVV). For example, based on the kinematic decomposition of (1), PVV dictates that the coarse scale virtual power equals that for the fine scale, i.e., $\delta\mathrm{P}^{\mathrm{int}}_{\mathrm{coarse}}=\mathbf{P}:\delta\dot{\mathbf{F}}^T+\mathbf{Q}\,\vdots\,\delta\dot{\mathbf{G}}$, where the coarse scale nominal stress, $\mathbf{P}$, and second-order stress, $\mathbf{Q}$, are defined in terms of distributions of boundary tractions, $\mathbf{t}_o$, and body forces, $\rho_o\mathbf{b}_o$, within the rSVE, i.e.,

$$\begin{aligned}\mathbf{P}^k &= \frac{1}{\Omega_o^{k+1}}\left(\int_{\Gamma_o^{k+1}}\mathbf{y}_o\otimes\mathbf{t}_o\,d\Gamma_o+\int_{\Omega_o^{k+1}}\mathbf{y}_o\otimes\rho_o\mathbf{b}_o d\Omega_o\right)\\ \mathbf{Q}^k &= \frac{1}{2\Omega_o^{k+1}}\left(\int_{\Gamma_o^{k+1}}\mathbf{t}_o\otimes\mathbf{y}_o\otimes\mathbf{y}_o\,d\Gamma_o+\int_{\Omega_o^{k+1}}\rho_o\mathbf{b}_o\otimes\mathbf{y}_o\otimes\mathbf{y}_o d\Omega_o\right)\end{aligned} \tag{2}$$

3.3. Scale Invariance of Angular Momentum

In standard first-order nonpolar continuum theories (at an arbitrary scale), balance of angular momentum imparts symmetry of the Cauchy stress tensor. In higher order theories, angular momentum is used to augment equations of motion with a balance between polar stresses and various aspects of material or substructure spin. Scale invariance of angular momentum in this multiscale framework establishes the lack of symmetry in the coarse scale Cauchy stress (i.e., $\mathbf{\Sigma}=(\mathbf{F}\cdot\mathbf{P})\det(\mathbf{F})^{-1}$) due to the distribution of finer scale tractions and long range gradients of deformation. Specifically, equation (3) expresses that the anti-symmetric part of the coarse scale Cauchy stress is equal to the sum of the anti-symmetric part of the first-moment of microinertia (first term on RHS) *and* a part of the second order stress projected onto the space of first order kinematics (second term on RHS), where $\mathbf{e}$ is the third order permutation tensor and ρ, $\mathbf{a}$, $\mathbf{y}$ are the mass density, acceleration, and position in the current configuration, respectively . Further implication of anti-symmetry of the coarse scale Cauchy stress to conservation of energy at the coarse scale is discussed in the next section.

$$\mathbf{e}:\mathbf{S} = \mathbf{e}:\left(\tfrac{1}{\Omega^x}\int_{\Omega^x}\mathbf{y}\otimes\rho\mathbf{a}d\Omega - \tfrac{1}{\det(\mathbf{F})}\mathbf{G}:\mathbf{Q}^T\right) \quad (3)$$

3.4. Scale invariance of total energy

The total energy in an rSVE of material should be invariant with respect to the scale of observation. In continuum thermomechanics, the two most common contributors to energy at any given scale are thermal and mechanical. Implementation of the developed framework to transitions between scales which are both represented by a continuum should assert that the total thermal and mechanical energy are equivalent at both scales of observation. However, it is possible that when transitioning to or from a scale that is treated in a discrete manner, for example molecular dynamics (MD) simulations, mechanical energy of finer scale fluctuations may translate into thermal energy at a continuum scale [10]. In continuum-to-continuum scale transitions, the total mechanical energy is consistent between both scales of observation if they exhibit scale invariance of momentum for all time. Thermal energy equivalence gives rise to a course scale definition of specific heat. Total energy invariance also dictates temperature changes due to dissipation of irreversible processes. The second-gradient kinematic decomposition results in the intermediate configuration energy equation (4) below for equivalence of internal energy. Note in particular the subtraction of the projected stress and the stress power associated with the second-order stress (second term on RHS), where the projected stress in the intermediate configuration, $\tilde{\mathbf{S}}^* = \det(\mathbf{F}_e)\left(\mathbf{F}_e^{-1}\cdot\mathbf{S}^*\cdot\mathbf{F}_e^{-T}\right)$, is the elastic-pull back of the projected Cauchy stress, $\mathbf{\Sigma}^* = \det(\mathbf{F})^{-1}\mathrm{sym}(\mathbf{G}:\mathbf{Q}^T)$, and $\mathbf{F}_e$ is the elastic part of the deformation gradient. Changes in thermal energy due to heat generation, $\overline{r}$, and flux, $\overline{\mathbf{q}}$, are captured by the last term on the right hand side of the equation

$$\tilde{\rho}\dot{\tilde{u}} = (\tilde{\mathbf{S}}-\tilde{\mathbf{S}}^*):\tilde{\mathbf{D}} + \tilde{\mathbf{Q}}\vdots L_v(\tilde{\mathbf{\Gamma}}) + \left(\overline{r} + \overline{\nabla}\cdot\overline{\mathbf{q}}\right)\det(\mathbf{F}_e) \quad (4)$$

3.5. Scale invariance of dissipation

A change in total energy of an rSVE can be partitioned into a change in free energy and an amount that has been dissipated. The change in free energy can be further decomposed into elastically recoverable and stored free energy. The actual energy dissipated during an irreversible process should be invariant with respect to the scale of observation. This principle is difficult to precisely adhere to in practice and it is possible to predict stresses and deformations at a coarse scale in a manner consistent with the deformation and distribution of stresses at a finer scale and totally complicit with all governing laws at both scales (conservation of mass, momentum, and energy, and non-negative dissipation) *without* an accurate representation of the dissipation at both scales. In a multiscale modeling strategy it is nonetheless desirable to pursue scale invariance of the dissipation on physical grounds. In the multiscale framework presented here, scale invariance of mechanical dissipation is expressed by equation (5) that requires the rate that energy is stored within the microstructure be equal to the "smeared" rate of energy storage for all sub-scale processes (first term RHS) and the energy stored due to inelastic incompatibility within the fine scale rSVE (last term RHS), i.e.,

$$\underbrace{\overline{\beta}^{(j)} * L_v(\overline{\xi}^{(j)})}_{\substack{\text{rate energy stored}\\ \text{to evolve microstructure}}} = \underbrace{\det(\mathbf{F}_e)\left(\tfrac{1}{\Omega^{k+1}}\int_{\Omega^{k+1}}\beta^{(k)} * \dot{\xi}^{(k)}d\Omega\right)}_{\substack{\text{rate energy stored in}\\ \text{sub fine-scale processes}}} + \underbrace{(\tilde{\mathbf{S}}-\tilde{\mathbf{S}}^*):\tilde{\mathbf{D}}_{in} + \tilde{\mathbf{Q}}\vdots L_v(\tilde{\mathbf{G}}_{in}) - \det(\mathbf{F}_e)\left(\tfrac{1}{\Omega^{k+1}}\int_{\Omega^{k+1}}\mathbf{s}:\mathbf{d}_{in}d\Omega\right)}_{\substack{\text{energy stored due to inelastic}\\ \text{incompatibility at fine scale}}} \quad (5)$$

where $\xi^{(k)}, \overline{\xi}^{(j)}$ are the internal state variables for the fine and course scales, respectively, and $\beta^{(k)}, \overline{\beta}^{(j)}$ are the corresponding thermodynamically conjugate driving forces. In (5), the fine scale inelastic power is expressed in the current configuration in terms of the fine scale Cauchy stress, $\mathbf{s}$, and inelastic part of the velocity gradient, $\mathbf{d}_{in}$, and pulled into the intermediate configuration by the determinant of the elastic part of the deformation gradient.

4. Concluding Remarks

Hierarchical scale transition approaches are limited in representation of localization of inelastic deformation (e.g., plasticity, damage); they are more appropriate for incipient localization, rather than post-bifurcation behavior. This owes to two features. First, it is required that the fine scale fluctuations do not have a correlation length on the order of the size of the volume element for which they are subjected to coarse-graining. Second, higher order moments of fluctuation would be required to rectify the kinematic complexity of post-localization behavior. One strategy would be to conduct a fine scale-resolved high degree of freedom simulation in regions where localization is indicated by incipient localization criteria embedded within a domain treated using various scales of the hierarchical formulation (like an “onion” being peeled back in layers). This requires restart of the solution from zero time. Another approach is to employ a fully concurrent multiscale modeling strategy at all points in which localization could occur, but this is quite costly. Yet another approach is to use a concurrent multiscale modeling strategy in which regions undergoing localization are successively refined and subjected to fine scale simulations. It may be possible to conceive of a hybrid approach in which hierarchical models at various scales are employed selectively in a concurrent scheme similar to that of Ghosh et al. [11] by imposing boundary conditions from a coarse scale solution subject to the requirement that the domain receiving enhanced resolution is large enough to ensure that stress and displacement redistribution due to localization has not yet substantially occurred.

Additionally, the hierarchical homogenization approach explicitly introduces length scales related to the adopted rSVE size as well as implicit length scales related to correlation lengths of dominant microstructure heterogeneity that are smaller than adopted finite rSVE domains. This emphasizes the importance of proper selection of the finite domain size to study at each scale transition. In some cases the finite domain size will be smaller than that necessary for a statistically representative volume (rRVE) such that stochastic analysis methods must be used with an rSVE.

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