NON-LOCAL MODELING OF MATERIAL FORCES DURING DAMAGE AND FRACTURE

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ABSTRACT
The purpose of this work is the formulation of models for the dynamics of continua with microstructure and material inhomogeneity. In particular, attention is focused on the balance relations and configurational fields for such continua obtained via invariance. Their formulation here is based on the Euclidean frame-indifference of the total energy balance together with the invariance of this balance with respect to changes of reference configuration. On this basis, one obtains additional balance relations for the microstructural fields as well as the dependence of the configurational fields on these. Combination of these results then facilitates the formulation of additional field relations pertaining to the case of a continuum with heterogeneous microstructure. In particular, this approach is applied in the current work to the case that the microstructure takes the form of microcracks or microvoids in the material whose effect on the material behaviour is isotropic and can be idealized as a continuum damage field.

1 INTRODUCTION

The behaviour of many materials of engineering interest (*e.g.*, metals, alloys, granular materials, composites, liquid crystals, polycrystals) is often influenced by an existing or emergent microstructure (*e.g.*, phases in multiphase materials, phase transitions, voids, microcracks, dislocation substructures, texture). In general, the components of such a microstructure have different material properties, resulting in a macroscopic material behaviour which is materially inhomogeneous. Attempts to incorporate this fact into the continuum modeling of such materials have lead to a number of approaches to and viewpoints on the issue, depending in part on the nature of the microstructure and corresponding inhomogeneity in question (*e.g.*, Noll [1]; Capriz [2]; Maugin [3]; Gurtin [4]). Beyond heterogeneous material properties, processes associated with the microstructure which are represented in the model by continuum fields (*e.g.*, damage and order parameter fields, director field) also contribute to configurational fields and processes. Such fields represent additional continuum degrees-of-freedom for which corresponding field relations must be formulated. Contigent on the premise that the corresponding processes contribute to energy flux and energy supply in the material, field relations for such degrees-of-freedom result from the Euclidean frame-indifference of the total rate-of-work (*e.g.*, Capriz [2]), or more generally from that of the total energy balance (*e.g.*, Capriz and Virga [5]; Svendsen [6], [7]). Once thermodynamically-consistent field relations and reduced constitutive relations have been obtained, one is in a position to formulate and solve initial-boundary-value problems. In the context of elastic material behaviour and thermodynamic equilibrium, such initial-boundary-value problems are often formulated variationally (*e.g.*, for elastic phase transitions: Ball and James [8]; for elastic liquid crystals: Virga [9]; for configurational fields in elastic materials: Podio-Guidugli [10]; see also Šilhavý [11], Chs. 13-21). Recently, it has been shown (*e.g.*, Ortiz and Repetto [12]; Miehe [13]; Carstensen *et al.* [14]) that direct variational methods for elastic materials can be carried over to the inelastic case with the help of a so-called incremental variational formulation. The purpose of this short work is the application of this incremental approach to the variational formulation of spatial balance relations as well as of configurational field and balance relations for a material inhomogeneous inelastic continuum containing a singular surface and isotropic damage. The formulation pursued here is general enough so that the damage may be of either brittle or ductile nature. For simplicity, the formulation in this work is restricted to isothermal and quasi-static conditions.

2 BASIC FORMULATION

Let E represent 3-dimensional Euclidean point space with translation vector space V, $B \subset E$ an arbitrary reference configuration of some material body containing a stationary coherent singular surface S, and $\boldsymbol{r} \in B$ the location of some material point in B. The time-dependent deformation or motion of the material body with respect to B and E in some time interval $I \subset \mathbb{R}^+$ takes the usual form $\boldsymbol{x}_t = \boldsymbol{\xi}(t, \boldsymbol{r}) \in E$ for all $t \in I$. Since S is coherent, $\boldsymbol{\xi}$ is continuous and piecewise continuously differentiable, implying that the jump $[\![\boldsymbol{\xi}]\!] := \boldsymbol{\xi}_+ - \boldsymbol{\xi}_-$ of $\boldsymbol{\xi}$ at S vanishes, *i.e.*, $[\![\boldsymbol{\xi}]\!] = \mathbf{0}$ holds. To account for the effects of non-local isotropic damage on the material behaviour, the standard continuum degrees of freedom as represented by $\boldsymbol{\xi}$ are complemented here by an additional time-dependent continuum field $d = \omega(t, \boldsymbol{r})$ on B taking values in the closed unit interval $[0, 1] \subset \mathbb{R}^+$. Basic kinematic quantities of interest include the material velocity $\dot{\boldsymbol{\xi}}(t, \boldsymbol{r}) \in V$ and the deformation gradient $\boldsymbol{F}(t, \boldsymbol{r}) := \nabla\boldsymbol{\xi}(t, \boldsymbol{r})$. Since S is stationary and $\boldsymbol{\xi}$ is continuous and piecewise continuously differentiable, the Hadamard lemma (*e.g.*, [11], Prop. 2.1.6) implies that $[\![\dot{\boldsymbol{\xi}}]\!] = \mathbf{0}$ and that $[\![\boldsymbol{F}]\!]$ is rank-one convex. For simplicity, attention is restricted here to the case that S is coherent with respect to ω as well, *i.e.*, $[\![\omega]\!] = \mathbf{0}$. The Hadamard lemma then yields $[\![\dot{\omega}]\!] = \mathbf{0}$ and $[\![\nabla\omega]\!]$ rank-one convex.

Assuming now that processes associated with the evolution of $\mathsf{x} := (\boldsymbol{\xi}, \omega)$ result in mechanical work being done in the system, the approach to the formulation of balance relations for materials with microstructure being pursued here is based on the total energy balance

$$\mathcal{E} = \overline{\int_P \psi}^{\,\cdot} + \int_P \delta - \int_{\partial P} \mathsf{f} \cdot \dot{\mathsf{x}} - \int_P \mathsf{s} \cdot \dot{\mathsf{x}} = 0 \tag{1}$$

for any part $P \subset B$ (*e.g.*, [15]). Note that volume dv and surface da measures are left out of the corresponding integral notations in this work for simplicity. Here, ψ represents the free energy density, δ the dissipation-rate density, F the generalized momentum flux density of normal to ∂B, and s the generalized momentum supply-rate density. Assuming in addition that the material with microstructure in question is materially inhomogeneous and behaves viscoelastically, the invariance of the total energy balance with respect to Euclidean observer (*e.g.*, [5]; [11], Ch. 6; [6]; [7]) together combined with the exploitation of the dissipation principle (*e.g.*, [11], Ch. 9; [6]; [7]) results in the field relations

$$\begin{aligned} \mathbf{0} &= \operatorname{div}(\partial_{\nabla\dot{\mathsf{x}}} r_{\rm I}) - \partial_{\dot{\mathsf{x}}} r_{\rm I} + \mathsf{s} \qquad &&\text{on } B \setminus S\,, \\ \mathbf{0} &= [\![\partial_{\nabla\dot{\mathsf{x}}} r_{\rm I}]\!]\boldsymbol{n} &&\text{on } S\,, \end{aligned} \tag{2}$$

(*e.g.*, [15]) and constitutive restriction $\mathsf{F} = \partial_{\nabla\dot{\mathsf{x}}} r_{\rm I}$ in terms of the rate potential $r_{\rm I} := \dot{\psi} + \chi_{\rm I}$. This potential is determined by the reduced forms $\psi = \psi(\mathsf{x}, \nabla\mathsf{x}, \boldsymbol{r})$ and $\chi_{\rm I} = \chi_{\rm I}(\mathsf{x}, \nabla\mathsf{x}, \dot{\mathsf{x}}, \nabla\dot{\mathsf{x}}, \boldsymbol{r})$ at any $\boldsymbol{r} \in B$ (for notational simplicity, we neglect the dependence of the constitutive relations on $\boldsymbol{r}$ in the notation until it becomes relevant). Note that material frame-indifference leads to a further reduction in the forms of ψ and $\chi_{\rm I}$ not accounted for here. The dissipation potential determines the residual constitutive form $\delta = \partial_{\dot{\mathsf{x}}}\chi_{\rm I} \cdot \dot{\mathsf{x}} + \partial_{\nabla\dot{\mathsf{x}}}\chi_{\rm I} \cdot \nabla\dot{\mathsf{x}} \geq \chi_{\rm I}$ of the dissipation-rate density δ, with equality holding in the rate-independent special case. Note that $\chi_{\rm I}$ is convex and minimal in its rate (*i.e.*, non-equilibrium) arguments $\dot{\mathsf{x}}$, $\nabla\dot{\boldsymbol{\xi}}$ and $\nabla\dot{\mathsf{x}}$, as well as non-negative.

3 RATE-BASED AND INCREMENTAL FORMULATIONS

For concreteness, the variational formulation to follow presumes a loading enviroment for the material under consideration of the displacement-traction type generalized to the current setting, *i.e.*, applying to x. Note that other such environments, *e.g.*, unilateral or bilateral contact (*e.g.*, [11], §13.3), can also be generalized to the current context and approach take here. As usual, the boundary

∂B of B is then divided into generalized displacement ∂B_x and generalized traction ∂B_f parts such that $\partial B = \partial B_x \cup \partial B_f$ and $\emptyset = \partial B_x \cap \partial B_f$ hold. By definition, f is compatible with $f = \partial_{\nabla\dot{x}} r_{\mathrm{I}}\, \boldsymbol{n}$ on ∂B_f, and vanishes on ∂B_x. Likewise, x is prescribed on ∂B_x. On this basis, consider the class of loading environments characterized by the non-conservative form

$$
-\int_B s\cdot\dot{x} - \int_{\partial B} f\cdot\dot{x} = \overline{\int_B w_s}^{\,\cdot} + \int_B (\partial_{\dot{x}}\chi_s\cdot\dot{x} + \partial_{\nabla\dot{x}}\chi_s\cdot\nabla\dot{x}) + \overline{\int_{\partial B_f} w_f}^{\,\cdot} + \int_{\partial B_f} \partial_{\dot{x}}\chi_f\cdot\dot{x} \tag{3}
$$

for the generalized power of external forces or rate of external work, holding for all kinematically-admissible x. Here, $w_s = w_s(x,\nabla x)$ and $w_f = w_f(x)$ represent direct generalizations of the bulk and surface potential energy densities for a conservative loading environment (*e.g.*, [11], §13.3) to the case of microstructure, while $\chi_s = \chi_s(x,\nabla x,\dot{x},\nabla\dot{x})$ and $\chi_f = \chi_f(x,\dot{x})$ represent corresponding dissipation potentials accounting for the effects of friction and other non-conservative loading processes in the bulk and on the boundary, respectively. In terms of the rate potentials $r_s := \dot{w}_s + \chi_s$ and $r_f := \dot{w}_f + \chi_f$ associated with the supply-rate and boundary-flux contributions, respectively, to the rate of external work, where $\delta_q f := \partial_q f - \mathrm{div}(\partial_{\nabla q} f)$ represents the variational derivative (*e.g.*, [16], Supplement 2.4C; [11], §13.3), (3) together with (2) yields

$$
\begin{aligned}
\mathbf{0} &= \delta_{\dot{x}}\, r && \text{on } B\setminus S\ ,\\
\mathbf{0} &= (\partial_{\nabla\dot{x}} r)\boldsymbol{n} + \partial_{\dot{x}} r_f && \text{on } \partial B_f\ ,\\
\mathbf{0} &= [\![\partial_{\nabla\dot{x}} r]\!]\boldsymbol{n} && \text{on } S\ ,
\end{aligned} \tag{4}
$$

where $r := r_{\mathrm{I}} + r_s$. In particular, $(4)_1$ implies that r is a null Lagrangian in the rates $\dot{x}$ (*e.g.*, [11], §13.6). As it turns out, these last relations represent the (rate) stationarity conditions of the (rate) functional

$$
R(x,\dot{x}) := \int_B r(x,\nabla x,\dot{x},\nabla\dot{x}) + \int_{\partial B_f} r_f(x,\dot{x}) \tag{5}
$$

with respect to B. This is a functional on the tangent bundle $T\mathcal{X}$ of the (infinite-dimensional) manifold $\mathcal{X}$ of all admissible states x. Note that this functional is bounded from above; indeed, in the context of (3), the energy balance (1) and result $\delta \geq \chi_{\mathrm{I}}$ imply $0 \geq R$, in particular via the convexity of r and r_f in their rate arguments. Again, equality holds in the rate-independent case. The vanishing of the variation of R with respect to admissible variations $\delta\,\dot{x}$ in the rates holding x fixed implies (4). In the tangent-bundle context, this represents the so-called fibre derivative of R on $T_x\mathcal{X}$ (*e.g.*, [16], Supplement 8.1B). In addition, one can show that the stability of rate stationary points of R is determined by the Hessian matrix of $\chi := \chi_{\mathrm{I}} + \chi_s$ with respect to its rates together with $\partial_{\dot{x}}(\partial_{\dot{x}}\chi_f)$. Since χ and χ_f are by definition convex in the rates, this matrix is positive-definite, R is minimal in the rates, and states satisfying (4) are stable in the rates.

Consider next the incremental form of the above rate-based variational formulation. Time-integration of R over the time interval $[t_n, t_{n+1}] \subset I$, rearrangement and forward-Euler approximation of the time-averages over $[t_n, t_{n+1}]$ yields the functional

$$
I_{n+1,n}(x_{n+1}) = \int_B \varphi_{n+1,n}(x_{n+1},\nabla x_{n+1}) + \int_{\partial B_f} \varphi_{f\,n+1,n}(x_{n+1}) \quad , \tag{6}
$$

where

$$
\begin{aligned}
\varphi_{n+1,n}(x_{n+1},\nabla x_{n+1}) &= \psi(x_{n+1},\nabla x_{n+1}) + w_s(x_{n+1},\nabla x_{n+1})\\
&+ t_{n+1,n}\,\chi(x_n,\nabla x_n, x_{n+1,n}/t_{n+1,n}, \nabla x_{n+1,n}/t_{n+1,n})\ ,\\
\varphi_{f\,n+1,n}(x_{n+1}) &= w_f(x_{n+1}) + \Delta t\,\chi_f(x_n, x_{n+1,n}/t_{n+1,n})\ ,
\end{aligned} \tag{7}
$$

represent the volume and surface density, respectively, of $I_{n+1,n}(\chi_{n+1})$, $t_{n+1,n} := t_{n+1} - t_n$, $\chi_{n+1,n} := \chi_{n+1} - \chi_n$ and likewise for $\nabla\chi$. Requiring the variation of $I_{n+1,n}(\chi_{n+1})$ with respect to χ_{n+1} to vanish for all admissible $\delta\chi_{n+1}$ results in the incremental form

$$\begin{aligned} \mathbf{0} &= \delta_{\chi_{n+1}}\varphi_{n+1,n} && \text{on } B \setminus S \ , \\ \mathbf{0} &= (\partial_{\nabla\chi_{n+1}}\varphi_{n+1,n})\boldsymbol{n} + \partial_{\chi_{n+1}}\varphi_{f\,n+1,n} && \text{on } \partial B_f \ , \\ \mathbf{0} &= [\![\partial_{\nabla\chi_{n+1}}\varphi_{n+1,n}]\!]\boldsymbol{n} && \text{on } S \ , \end{aligned} \tag{8}$$

of the system (4). Analogous to r being a null Lagrangian in $\dot{\chi}$ on the basis of $(4)_1$, note that $(8)_1$ implies that $\varphi_{n+1,n}$ is a null Lagrangian in χ_{n+1} (*e.g.*, [11], §13.6). Like for the canonical free energy, one can show that $I_{n+1,n}(\chi_{n+1})$ is a (monotonically) non-increasing function (*e.g.*, [15]), and so a possible Liapunov function for the processes of interest (*e.g.*, [11], Ch. 15).

4 VARIATIONAL FORMULATION OF CONFIGURATIONAL FIELDS AND RELATIONS

The results of the variational formulation from the last section were obtained by varying the fields holding the reference configuration B of the material under consideration fixed. As is well-known (*e.g.*, [11], §14.5; [10]), variations of the reference configuration at fixed fields yield in the elastic context variational forms of configurational fields and balance relations. The purpose of this section is to derive these in the current setting with respect to the incremental functional $I_{n+1,n}(\chi_{n+1})$ from (6). To do this, we reintroduce the dependence of the constitutive relations on $\boldsymbol{r} \in B$ and consider a smooth variation of B as represented by a one-parameter family $\boldsymbol{\lambda}_\tau : B \to B_\tau \mid \boldsymbol{r} \mapsto \boldsymbol{r}_\tau = \boldsymbol{\lambda}_\tau(\boldsymbol{r})$ of transformations of B which leave ∂B *fixed*. By definition, $\boldsymbol{r}_0 = \boldsymbol{\lambda}_0(\boldsymbol{r}) = \boldsymbol{r}$ and $\nabla\boldsymbol{\lambda}_0 = \mathbf{1}$. This one-parameter family induces the corresponding parameterized form [1]

$$\bar{I}(\tau) := \int_{\boldsymbol{\lambda}_\tau[B]} \varphi(\chi_\tau, \nabla\chi_\tau, \boldsymbol{r}_\tau) + \int_{\partial B_f} \varphi_f(\chi, \boldsymbol{r}) \tag{9}$$

of $I_{n+1,n}$, where $\chi_\tau := \chi \circ \boldsymbol{\lambda}_\tau^{-1}$. Pulling (9) back to B then yields

$$\bar{I}(\tau) = \int_B \varphi(\chi, \nabla\chi_\tau \circ \boldsymbol{\lambda}_\tau, \boldsymbol{\lambda}_\tau(\boldsymbol{r}))\,\det(\nabla\boldsymbol{\lambda}_\tau) + \int_{\partial B_f} \varphi_f(\chi, \boldsymbol{r}) \quad , \tag{10}$$

and so the result

$$\partial_\tau \bar{I}|_{\tau=0} = \int_B \partial_{\nabla\chi}\varphi \cdot \partial_\tau(\nabla\chi_\tau \circ \boldsymbol{\lambda}_\tau)|_{\tau=0} + \partial_{\boldsymbol{r}}\varphi \cdot \boldsymbol{v} + \varphi\,\mathbf{1} \cdot \nabla\boldsymbol{v} \tag{11}$$

for its variation with respect to τ, where $\boldsymbol{v} := (\partial_\tau\boldsymbol{\lambda}_\tau)|_{\tau=0}$. Since $\boldsymbol{\lambda}_\tau$ leaves the boundary ∂B of B fixed by definition, note that $\boldsymbol{v}$ vanishes on ∂B. Now, from the result $\mathbf{0} = \partial_\tau(\nabla\chi) = \partial_\tau(\nabla\chi_\tau \circ \boldsymbol{\lambda}_\tau)\,(\nabla\boldsymbol{\lambda}_\tau) + (\nabla\chi_\tau \circ \boldsymbol{\lambda}_\tau)\,\partial_\tau(\nabla\boldsymbol{\lambda}_\tau)$, we obtain $\partial_\tau(\nabla\chi_\tau \circ \boldsymbol{\lambda}_\tau)|_{\tau=0} = -(\nabla\chi)\,(\nabla\boldsymbol{v})|_{\tau=0}$. Substituting this into (11), it reduces to

$$\begin{aligned} \partial_\tau \bar{I}|_{\tau=0} &= \int_B \partial_{\boldsymbol{r}}\varphi \cdot \boldsymbol{v} + \{\varphi\mathbf{1} - (\nabla\chi)^{\mathrm{T}}(\partial_{\nabla\chi}\varphi)\} \cdot \nabla\boldsymbol{v} \\ &= \int_B \{\partial_{\boldsymbol{r}}\varphi - \operatorname{div}[\varphi\mathbf{1} - (\nabla\chi)^{\mathrm{T}}(\partial_{\nabla\chi}\varphi)]\} \cdot \boldsymbol{v} \\ &\quad - \int_S [\![\varphi\mathbf{1} - (\nabla\chi)^{\mathrm{T}}(\partial_{\nabla\chi}\varphi)]\!]\boldsymbol{n} \cdot \boldsymbol{v} \ , \end{aligned} \tag{12}$$

[1] Dropping the e and s subscripts for the moment.

again since $\boldsymbol{v}$ vanishes on ∂B. Consequently, the requirement that $I_{n+1,n}$ be independent of (compatible) change of reference configuration, *i.e.*, that $\partial_\tau \bar{I}_{n+1,n}|_{\tau=0}$ vanish for all variations $\boldsymbol{v}$ leaving ∂B fixed, then implies

$$
\begin{aligned}
\mathbf{0} &= \operatorname{div} \boldsymbol{E}_{n+1,n} - \partial_{\boldsymbol{r}} \varphi_{n+1,n} && \text{on } B \setminus S\,, \\
\mathbf{0} &= [\![\boldsymbol{E}_{n+1,n}]\!] \boldsymbol{n} && \text{on } S\,.
\end{aligned}
\tag{13}
$$

Here,

$$
\begin{aligned}
\boldsymbol{E}_{n+1,n} &:= \varphi_{n+1,n}\,\mathbf{1} - (\nabla \chi_{n+1})^{\mathrm{T}} (\partial_{\nabla \chi_{n+1}} \varphi_{n+1,n}) \\
&= \varphi_{n+1,n}\,\mathbf{1} - (\nabla \boldsymbol{\xi}_{n+1})^{\mathrm{T}} (\partial_{\nabla \boldsymbol{\xi}_{n+1}} \varphi_{n+1,n}) - (\nabla \omega_{n+1}) \otimes (\partial_{\nabla \omega_{n+1}} \varphi_{n+1,n})
\end{aligned}
\tag{14}
$$

represents the generalized total Eshelby or configurational stress tensor in the context of the incremental formulation.

The generalized form (14) for the configurational stress is formally analogous to that for the elastic case (*e.g.*, in the standard context: [3]; in the microstructural context: [7]) in which $\boldsymbol{E}$ is determined by the free energy density ψ. Indeed, the role of ψ in the elastic case is played in the current inelastic context by $\varphi_{n+1,n}$. Finally, note that, if the material behaviour is homogeneous, then $\varphi_{n+1,n}$ is translationally invariant, *i.e.*, $\varphi_{n+1,n}(\chi_{n+1}, \nabla\chi_{n+1}, \boldsymbol{r} + \boldsymbol{a}) = \varphi_{n+1,n}(\chi_{n+1}, \nabla\chi_{n+1}, \boldsymbol{r})$ holds for all $\boldsymbol{a} \in V$. In this case, $\partial_{\boldsymbol{r}} \varphi_{n+1,n}$ vanishes, and $(13)_1$ reduces to $\mathbf{0} = \operatorname{div} \boldsymbol{E}_{n+1,n}$. In this case, the total Eshelby stress tensor is analogous to a null divergence (*e.g.*, [17]; [11], §13.6).

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