COMPUTATION OF MATERIAL FORCES BASED ON A GRADIENT-ENHANCED MIXED VARIATIONAL FORMULATION

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Summary. Configurational (or material) forces are computed based on a previously derived thermodynamically consistent definition of material forces, in conjunction with a gradient-enhanced constitutive theory. The primary problem solved for is based on a mixed variational formulation. Under the proposed mixed formulation, no nodal smoothing of internal variables for the computation of material forces is required at the post-processing. Results are shown in terms of energetic quantities which stem from the computed material forces. The mesh sensitivity of the latter quantities is examined and compared to respective results based on local constitutive theory in a "standard" displacements-based variational formulation.

1 INTRODUCTION

It is rather convenient in terms of computational cost and model development to compute configurational forces for inelasticity via a "conventional" displacement-based variational formulation. However, under such discontinuous representation of the internal variables field, simulation results of problems which involve sources of numerical singularity (e.g. a crack-tip) exhibit "pathological" mesh dependence, see e.g. Tillberg et al.[1]. In addition, as shown in Menzel et al.[2], "no" accuracy is gained from constructing a mixed variational formulation in terms of the displacements and the internal variables field.

In this work, configurational forces are computed based on a gradient-enhanced constitutive theory. The primary problem solved for comprises a mixed variational formulation in terms of the displacements along with a gradient-related field. The gradient-enhanced constitutive theory, in conjunction with the continuous approximation of the gradient field, provide sufficient regularity for the computation of material forces, especially for larger values of the internal regularization parameter.

2 VARIATIONAL FORMULATION IN MIXED-DUAL FORMAT

The primary problem comprises that of determining the fields $\boldsymbol{u}(\boldsymbol{x},t)$, $\underline{\boldsymbol{\xi}}(\boldsymbol{x},t)$, $\underline{k}(\boldsymbol{x},t)$, $\underline{\boldsymbol{\kappa}}^{\mathrm{di}}(\boldsymbol{x},t)$ that satisfy[‡]

$$-\boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}],\underline{k})\cdot\boldsymbol{\nabla}=\boldsymbol{0} \quad \text{in } \Omega, \tag{1}$$

$$\underline{\boldsymbol{\kappa}}^{\mathrm{en}}(\boldsymbol{\epsilon}[\boldsymbol{u}],\underline{k})+\underline{\boldsymbol{\kappa}}^{\mathrm{di}}-\underline{\boldsymbol{\xi}}\cdot\boldsymbol{\nabla}=\underline{\boldsymbol{0}} \quad \text{in } \Omega, \tag{2}$$

$$\underline{\boldsymbol{g}}[\underline{k}]-\underline{\boldsymbol{g}}(\underline{\boldsymbol{\xi}})=\underline{\boldsymbol{0}} \quad \text{in } \Omega, \tag{3}$$

$$\underline{k}-\Delta t\frac{\partial\phi^{*}}{\partial\underline{\boldsymbol{\kappa}}^{\mathrm{di}}}(\underline{\boldsymbol{\kappa}}^{\mathrm{di}})={}^{n}\underline{k} \quad \text{in } \Omega, \tag{4}$$

where $\underline{k}$ denotes the internal variables structure, $\underline{\boldsymbol{\kappa}}^{\mathrm{di}}$ is the dissipative stress field, $\phi^{*}(\underline{\boldsymbol{\kappa}}^{\mathrm{di}})$ is a dissipation functional in terms of $\underline{\boldsymbol{\kappa}}^{\mathrm{di}}$, $\boldsymbol{\epsilon}[\boldsymbol{u}]=[\boldsymbol{u}\otimes\boldsymbol{\nabla}]^{\mathrm{sym}}$, and, $\underline{\boldsymbol{g}}[\underline{k}]\overset{\mathrm{def}}{=}\underline{k}\otimes\boldsymbol{\nabla}$. The Coleman-type equations read

$$\boldsymbol{\sigma}\overset{\mathrm{def}}{=}\frac{\partial\psi}{\partial\boldsymbol{\epsilon}}, \quad \underline{\boldsymbol{\kappa}}^{\mathrm{en}}\overset{\mathrm{def}}{=}\frac{\partial\psi}{\partial\underline{k}}, \quad \underline{\boldsymbol{\xi}}\overset{\mathrm{def}}{=}\frac{\partial\psi}{\partial\underline{\boldsymbol{g}}}, \tag{5}$$

where the corresponding free energy for a gradient-enhanced dissipative material is introduced as

$$\psi(\boldsymbol{\epsilon},\underline{k},\underline{\boldsymbol{g}})=\psi^{\mathrm{loc}}(\boldsymbol{\epsilon},\underline{k})+\psi^{\mathrm{gra}}(\underline{\boldsymbol{g}}). \tag{6}$$

The constitutive equation for $\underline{\boldsymbol{g}}(\underline{\boldsymbol{\xi}})$ in (3) is expressed as

$$\underline{\boldsymbol{g}}(\underline{\boldsymbol{\xi}})=\frac{\partial\psi^{*,\mathrm{gra}}}{\partial\underline{\boldsymbol{\xi}}} \tag{7}$$

where $\psi^{*,\mathrm{gra}}(\underline{\boldsymbol{\xi}})$ is obtained via a Legendre transformation w.r.t. the gradient variable $\underline{\boldsymbol{g}}$.

Employing the principle of virtual work and Green-Gauss theorem on (1)–(4) results in the time-discrete *semi-dual* weak format of finding $\boldsymbol{u}$, $\underline{\boldsymbol{\xi}}$ such that

$$R_{\mathrm{u}}(\boldsymbol{u},\underline{\boldsymbol{\xi}};\delta\boldsymbol{u})=\int_{\Omega}\boldsymbol{\sigma}(\boldsymbol{\epsilon}[\boldsymbol{u}],\underline{k}\{\boldsymbol{\epsilon}[\boldsymbol{u}],\underline{\boldsymbol{\chi}}[\underline{\boldsymbol{\xi}}]\}):\boldsymbol{\epsilon}[\delta\boldsymbol{u}]\,\mathrm{d}\Omega-l^{(u)}(\delta\boldsymbol{u})=0, \tag{8}$$

$$R_{\xi}(\boldsymbol{u},\underline{\boldsymbol{\xi}};\delta\underline{\boldsymbol{\xi}})=\int_{\Omega}\left[-\underline{k}\{\boldsymbol{\epsilon}[\boldsymbol{u}],\underline{\boldsymbol{\chi}}[\underline{\boldsymbol{\xi}}]\}\star\underline{\boldsymbol{\chi}}[\delta\underline{\boldsymbol{\xi}}]-\underline{\boldsymbol{g}}(\underline{\boldsymbol{\xi}})\star\delta\underline{\boldsymbol{\xi}}\right]\mathrm{d}\Omega-l^{(\xi)}(\delta\underline{\boldsymbol{\xi}})=0, \tag{9}$$

for suitable test functions $\delta\boldsymbol{u}$, $\delta\underline{\boldsymbol{\xi}}$. The linear forms (external work) in (8), (9) read

$$l^{(u)}(\delta\boldsymbol{u})=\int_{\Gamma}\bar{\boldsymbol{t}}_{\mathrm{p}}\cdot\delta\boldsymbol{u}\,\mathrm{d}\Gamma \quad , \quad l^{(\xi)}(\delta\underline{\boldsymbol{\xi}})=-\int_{\Gamma}\bar{\underline{k}}_{\mathrm{p}}\star[\delta\underline{\boldsymbol{\xi}}\cdot\boldsymbol{n}]_{\mathrm{p}}\,\mathrm{d}\Gamma. \tag{10}$$

Moreover, choosing to satisfy the weak form of (2) and (4) in a strong sense leads to the "local" equations

$$\underline{\boldsymbol{R}}_{\mathrm{L}}(\boldsymbol{u},\underline{\boldsymbol{\xi}},\underline{k})=\underline{k}-\Delta t\frac{\partial\phi^{*}}{\partial\underline{\boldsymbol{\kappa}}^{\mathrm{di}}}(\underline{\boldsymbol{\chi}}[\underline{\boldsymbol{\xi}}]-\underline{\boldsymbol{\kappa}}^{\mathrm{en}}(\boldsymbol{\epsilon}[\boldsymbol{u}],\underline{k}))-{}^{n}\underline{k}=\underline{\boldsymbol{0}}. \tag{11}$$

[‡]For brevity, all discussions on boundary conditions and trial and test spaces that naturally complete the definition of the strong and weak formats, respectively, are omitted.

3 CONFIGURATIONAL FORCES

In Runesson et al.[3], it was shown that the mechanical dissipation $\mathcal{D}$, may be split into two parts, the configurational $\mathcal{D}^{\mathrm{CONF}}$ and the material dissipation part $\mathcal{D}^{\mathrm{MAT}}$. Partial variation of $\mathcal{D}$ and parametrization $\mathrm{d}\dot{\boldsymbol{X}} = \overline{W}(\boldsymbol{X})\,\mathrm{d}\dot{\boldsymbol{a}}$ of the update in the initial (undeformed) configuration result in $\boldsymbol{\mathcal{G}} \cdot \mathrm{d}\dot{\boldsymbol{a}}$, where $\boldsymbol{\mathcal{G}}$ is a generalized crack driving force , $\dot{\boldsymbol{a}}$ is equivalent to a crack advance rate and $\overline{W}$ is a scaling function of the configurational motion. In this context, the two parts of the total configurational force for gradient-enhanced constitutive theory[‡] can be written as
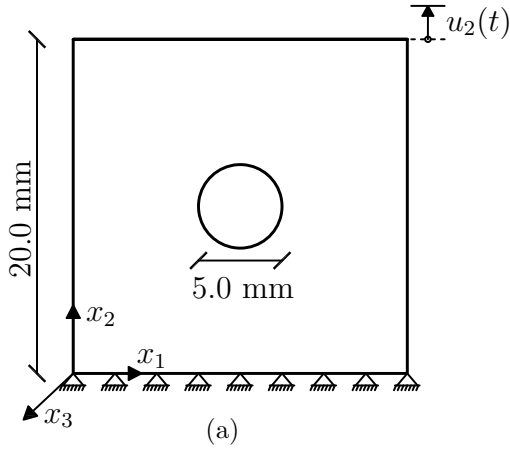
$$\boldsymbol{\mathcal{G}}^{\mathrm{CONF}} = \int_{\Omega} -(\boldsymbol{\nabla}\overline{W}) \cdot \boldsymbol{\Sigma}\,\mathrm{d}\Omega, \tag{12}$$

$$\boldsymbol{\mathcal{G}}^{\mathrm{MAT}} = \int_{\Omega} \left[-\frac{\partial\psi}{\partial\underline{k}} \star [\underline{k} \otimes \boldsymbol{\nabla}] - \frac{\partial\psi}{\partial\underline{g}} \star [\underline{g} \otimes \boldsymbol{\nabla}] \right] \overline{W}\,\mathrm{d}\Omega, \tag{13}$$

where $\boldsymbol{\Sigma} \stackrel{\mathrm{def}}{=} \psi\boldsymbol{I} - \boldsymbol{H}^{\mathrm{T}}\cdot\boldsymbol{\sigma}$ is Eshelby's stress tensor in small strains setting and $\boldsymbol{H} = [\boldsymbol{u}\otimes\boldsymbol{\nabla}]$.

4 NUMERICAL EXAMPLE

The smooth interphase problem defined by a square plate with centric hole subjected to prescribed displacement $u_2 = 0.1$ mm of the upper edge, see Fig. 1a, is outlined next.

Young's modulus, E [GPa]	200
Poisson's ratio, ν	0.3
Yield stress, σ_{y} [MPa]	200
Characteristic stress, σ_{C} [MPa]	200
Gradient hardening modulus, H_{g} [GPa]	20
Viscoplastic time parameter, t_* [s]	0.01
Total time of direct motion, t^{TOTAL} [s]	0.05

(a) (b)

Figure 1: (a) Geometry and Dirichlet boundary conditions on the displacements.
(b) Material parameters that enter the gradient-enhanced viscoplastic constitutive model.

A gradient-enhanced Bingham's perfect viscoplastic model is used, i.e. $\underline{k} \equiv \boldsymbol{\epsilon}^{\mathrm{p}}$. The *semi-dual* free energy of the model reads

$$\varphi(\boldsymbol{\epsilon}, \boldsymbol{\epsilon}^{\mathrm{p}}, \boldsymbol{\xi}) = \underbrace{\frac{1}{2}\left[\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^{\mathrm{p}}\right] : \mathbf{E} : \left[\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^{\mathrm{p}}\right]}_{\psi^{\mathrm{loc}}(\boldsymbol{\epsilon}, \boldsymbol{\epsilon}^{\mathrm{p}})} - \underbrace{\frac{1}{2H_{\mathrm{g}}l_{\mathrm{s}}^2}|\boldsymbol{\xi}|^2}_{\psi^{*,\mathrm{gra}}(\boldsymbol{\xi})}. \tag{14}$$

[‡]In local theory, (12) remains unchanged, while the latter term on the RHS of (13) vanishes.

The dual dissipation potential $\phi^*(\boldsymbol{\kappa}^{\mathrm{di}})$ is defined here by

$$\phi^*(\boldsymbol{\kappa}^{\mathrm{di}}) = \frac{1}{t_*}\eta(F(\boldsymbol{\kappa}^{\mathrm{di}})) \quad , \quad F(\boldsymbol{\kappa}^{\mathrm{di}}) = \sqrt{\frac{3}{2}}|\boldsymbol{\kappa}_{\mathrm{dev}}^{\mathrm{di}}| - \sigma_{\mathrm{y}} \quad , \quad \eta(F) = \frac{1}{2}\frac{\langle F\rangle^2}{\sigma_{\mathrm{c}}}, \qquad (15)$$

where all material parameters are introduced in the table of Fig. 1b. In Figs. 2a and 2b, results in terms of energy release rates due to a virtual expansion of the hole are compared for different values of the length scale parameter l_{s}.
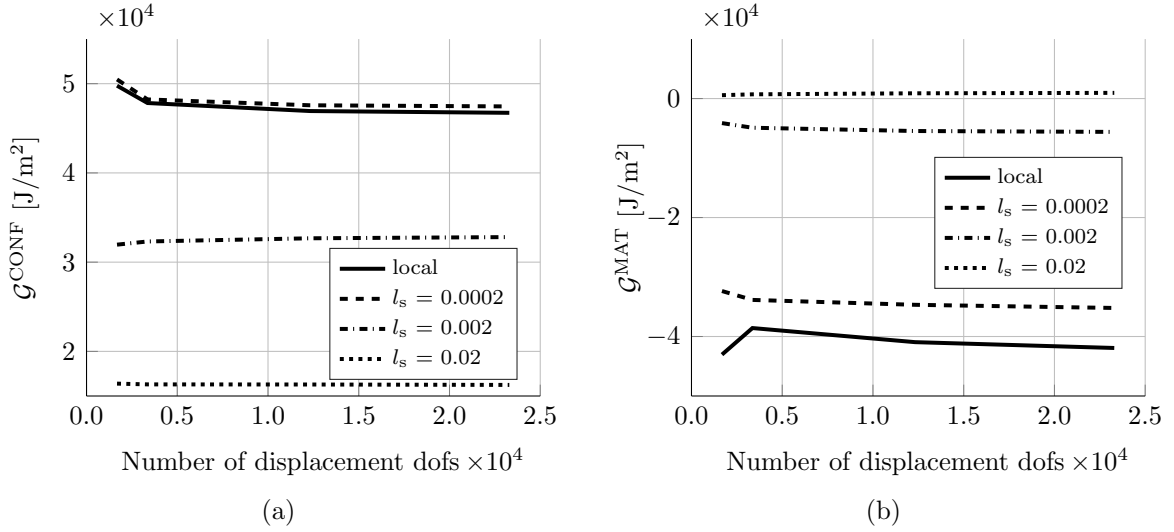

Figure 2: Energy release rates for expanding hole. (a) Configurational part $\mathcal{G}^{\mathrm{CONF}}$. (b) Material dissipation part $\mathcal{G}^{\mathrm{MAT}}$.

5   CONCLUSIONS

Configurational forces are computed based on a gradient-enhanced mixed variational formulation. Unconditional convergence of energy release rates for finite values of the regularization parameter is achieved. The behavior of a pure local constitutive model is resembled as we let the regularization parameter tend to zero and for appropriate choice of gradient-related boundary conditions.

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