

Numerical approximation of incremental infinitesimal gradient plasticity

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SUMMARY

We investigate a representative model of continuum infinitesimal gradient plasticity. The formulation is an extension of classical rate-independent infinitesimal plasticity based on the additive decomposition of the symmetric strain tensor into elastic and plastic parts. It is assumed that dislocation processes contribute to the storage of energy in the material whereby the curl of the plastic distortion appears in the thermodynamic potential and leads to an additional nonlocal backstress tensor. The formulation is cast into a numerical framework by a saddle point approximation of the corresponding minimization problem in each incremental loading step. This allows one to reformulate the (nonlocal) dissipation inequality to a point-wise flow rule and yields a solution scheme, which is a direct extension of the standard approach in classical plasticity. Our numerical results show the regularizing effects of the additional physically motivated terms. Copyright © 2008 John Wiley & Sons, Ltd.

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1. INTRODUCTION

This article addresses the numerical analysis of a *geometrically linear isotropic gradient plasticity* model. There is an abundant literature on gradient plasticity formulations, in most cases letting the yield stress K_0 depend also on some higher derivative of a scalar measure of accumulated plastic distortion [1–3]. Experimentally, the dependence of the yield stress on plastic gradients is well documented (see, e.g. [4]), and several experimental facts testify to the length scale dependence of materials. The *Hall–Petch scaling*, for instance, relates the grain size in polycrystals to the yield stress in the form $K_0 = K_0^0 + k^+/\sqrt{\text{grain size}}$.

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Similarly, the *Taylor scaling* relates the yield stress K_0 to the dislocation density qualitatively by $K_0 = K_0^0 + k^+ |\text{curl}(\mathbf{F}_p)|$, where $\mathbf{F}_p$ is the incompatible intermediate configuration appearing in the multiplicative decomposition [5] and $\text{curl}\mathbf{F}_p$ is a measure for the defect density.[‡]

It is also known that the thinner the grains, the stiffer the material gets. As a rule one may therefore say that the smaller the sample, the stiffer it gets (while unbounded stiffness must be excluded from atomistic calculations).

From a numerical point of view, the incorporation of plastic gradients may also serve the purpose of removing the mesh sensitivity, ubiquitous in the softening case, or, more difficult to observe numerically, already in classical Prandtl–Reuss plasticity (shear bands and slip lines with ill-defined band width, as, for example, in the case of a plate with a hole under uniform tension [7]).

The incorporation of a plastic length scale, which is a natural by-product of gradient plasticity, has the potential to remove the mesh sensitivity. The presence of the internal length scale should cause the localization zones to have a finite width. It allows for the analysis of failure problems in which strain localization into shear bands occurs. However, the actual plastic length scale of a material is difficult to determine experimentally and theoretically, and thus it remains an open question how to determine the additionally appearing material constants. Moreover, how the width of the shear bands depends on the characteristic length is also not entirely clear.

Models similar in spirit to our formulation may be found in [8, 9]. Although gradient plasticity seems to be of high current interest [10–14] we have not been able to locate many rigorous mathematical studies of the time continuous higher gradient plasticity problem, apart for Reddy *et al.* [15], treating a geometrically linear model of Gurtin and Anand [12], which is substantially different from our proposal.[§] A rigorous mathematical study of a rate-independent problem with full gradient regularization, although coming from ferroelasticity, is presented in [16, 17].

Gurtin includes $\text{curl}(\mathbf{F}_p)$ in the free energy and takes free variations with respect to $\mathbf{F}_p$, leading to a model with additional balance equations for microforces, similar, e.g. to a Cosserat- or Toupin–Mindlin-type model. We refer to [7, 18] for a model including plasticity and Cosserat effects. In modification of Gurtin’s approach, the plastic distortion $\mathbf{F}_p$, and thus $\text{curl}(\mathbf{F}_p)$ in [19, 20], is treated as an inner variable included only in the thermodynamic potential, leading to a system of evolution equations for $\mathbf{F}_p$ of degenerated parabolic type.

In [21] the time-incremental finite-strain problem is investigated. It is shown that once the update potential for one time step is established and known to be properly coercive and polyconvex as a function of $\mathbf{F}_e$ in the multiplicative decomposition of the deformation gradient, then adding a regularizing term depending only on $\text{curl}(\mathbf{F}_p)$ is indeed enough to show the existence of minimizers for the new deformation and the new plastic variable.[¶]

[‡]Note that we use the transpose of Gurtin’s definition of the curl operator for second-order tensors, i.e. curl acts row-wise such that $\text{curl} D\varphi = 0$. Formulas given in [6] do not obtain for this definition.

[§]In Reddy’s analytical treatment of the corresponding infinitesimal model, strong assumptions on the presence of the full plastic strain rate gradient (instead of the curl) are introduced depending on the yield stress of the plastic gradients (isotropic hardening) in order to show existence and uniqueness. His model features *a priori* purely symmetric plastic strains. Such a model is called ‘irrotational’; it does not allow for plastic spin. Local kinematic hardening is not considered.

[¶]It is noteworthy that the update problem in [21] is a two-field minimization problem for the deformation and plastic distortion $(\varphi, \mathbf{F}_p)$ in the spirit of a micromorphic model [22] with a very special coupling between the different fields φ and $\mathbf{F}_p$. Polyconvexity in $\mathbf{F}_e$ alone is not sufficient to obtain existence by Ball’s method since $\mathbf{F}_e$ is not a gradient, but the term $\text{curl}(\mathbf{F}_p)$ provides additional compactness in the spirit of Murat–Tartar’s method.

Adding a $\text{curl}(\mathbf{F}_p)$ -related term to the time-incremental problem has also been suggested in [23] for the description of subgrain dislocation structures. It therefore seems necessary to investigate the general structure of this class of gradient plasticity models. Here our interest mainly concerns the regularizing power of these models. Focussing therefore on localization limiters we investigate a well-posed plasticity model that includes the dislocation energy density and local linear Prager kinematic hardening. In the large-scale (classical) limit of vanishing plastic length scale our model turns into Prandtl–Reuss plasticity with linear kinematic hardening.

As far as classical rate-independent perfect elasto-plasticity is concerned, we remark that global existence for the displacement has been shown only in a very weak, measure-valued sense, while the stresses could be shown to remain in $L_2(\Omega, \text{Sym}(3))$. For these results we refer, for example, to [24–26]. If hardening or viscosity is added, then global classical solutions are found, see, e.g. [27–29]. A complete theory for the classical rate-independent case remains elusive; see also the remarks in [25]. It is therefore hoped that including plastic gradients in the formulation will regularize the problem and lead to a well-posed model. This is what is shown in [20].

In the small strain gradient plasticity model proposed in [20] the plastic distortion $\mathbf{p}$ is in general not symmetric. Imposing certain form-invariance conditions (invariance of the referential, intermediate and spatial configuration under superposed rotations) on the thermodynamic potential shows that the local kinematical backstress in the linearized regime can depend only on $\text{sym}(\mathbf{p})$, while the nonlocal backstress depends on the (in general, nonsymmetric) expression $\text{curl}(\text{curl}(\mathbf{p}))$.

However, excluding plastic spin (i.e. $\text{skew}(\mathbf{F}_p^{-1}\dot{\mathbf{F}}_p)$) as a constitutive choice (no spin assumption, see [30, 31]) leads, after linearization, to a symmetric plastic distortion rate ($\dot{\mathbf{p}} \in \text{Sym}(3)$), thereby considering only the symmetric part of the relative (elastic) stress $\boldsymbol{\alpha} = \boldsymbol{\sigma} - \mathbb{D}\mathbf{p} - \text{curl}(\text{curl}(\mathbf{p}))$. Taking symmetric initial values for the plastic distortion $\mathbf{p}$, it is thus possible to consider a gradient plasticity model in which only symmetric plastic strains occur. This is what we do here; we may rename $\boldsymbol{\varepsilon}_p = \text{sym}\mathbf{p}$.

One of our main objectives is to show that our gradient plasticity model can simply be obtained by augmenting the classical energy contribution with a nonlocal term. In addition, the classical concept of a discretization with the help of the flow rule can still be used in our proposed mixed formulation.

This article is organized as follows. In Section 2, we introduce the model step by step, where we discuss, in particular, the relation of the flow rule and dissipation inequality for the nonlocal model. Then, in Section 3, we consider the incremental model and we derive a mixed approximation in space. It is shown that this problem corresponds to a constrained minimization problem, and we derive the characterizing KKT-system. For this KKT-system an iterative numerical scheme is developed in Section 4 by linearizing the flow rule in every step, where each iteration step itself is a non-linear problem (solved by a nonsmooth Newton method). Finally, in Section 5 we present a numerical study, which shows that the proposed scheme is a robust and efficient solution method. Moreover, the results clearly illustrate the regularization properties of the nonlocal method.

2. A REPRESENTATIVE MODEL FOR INFINITESIMAL NONLOCAL PLASTICITY

We develop a model for nonlocal plasticity in three stages: beginning with infinitesimal perfect plasticity (which is not well posed in the primal setting), the model is first regularized by including local kinematic hardening. In the last step it is extended by a nonlocal term that depends on the curl of the plastic distortion.

2.1. Data

Let $\Omega \subset \mathbf{R}^3$ be the reference configuration, and let $\Gamma_D \cup \Gamma_N = \partial\Omega$ be a decomposition of the boundary. The outer unit normal vector on the boundary is denoted by $\mathbf{n}(\mathbf{x})$. Let $[0, T]$ be a fixed time interval. We prescribe a displacement vector

$$\mathbf{u}_D: \Gamma_D \times [0, T] \longrightarrow \mathbf{R}^3$$

for the essential boundary conditions on Γ_D and a load functional

$$\ell(t, \delta \mathbf{u}) = \int_{\Omega} \mathbf{b}(t) \cdot \delta \mathbf{u} \, d\mathbf{x} + \int_{\Gamma_N} \mathbf{t}_N(t) \cdot \delta \mathbf{u} \, da$$

depending on body force densities and traction force densities

$$\mathbf{b}: \Omega \times [0, T] \longrightarrow \mathbf{R}^3, \quad \mathbf{t}_N: \Gamma_N \times [0, T] \longrightarrow \mathbf{R}^3$$

In all cases below we assume that the data are sufficiently smooth.

Let $\text{Sym}(3) = \{\boldsymbol{\tau} \in \mathbf{R}^{3,3}: \boldsymbol{\tau}^T = \boldsymbol{\tau}\}$ be the set of symmetric matrices. The elastic material properties (in the infinitesimal model) are given through the isotropic elasticity tensor $\mathbb{C}: \text{Sym}(3) \longrightarrow \text{Sym}(3)$ defined by $\mathbb{C}: \boldsymbol{\varepsilon} = 2\mu\boldsymbol{\varepsilon} + \lambda \text{trace}(\boldsymbol{\varepsilon})\mathbb{1}$, depending on the Lamé constants λ, μ . On $\text{Sym}(3)$, we assume that the elasticity tensor is symmetric and positive definite. For a displacement vector $\mathbf{u}$, the linearized strain tensor is denoted by $\boldsymbol{\varepsilon}(\mathbf{u}) = \text{sym}(D\mathbf{u})$.

We restrict ourselves to von Mises plasticity $\phi(\boldsymbol{\sigma}) = |\text{dev}(\boldsymbol{\sigma})| - K_0$ depending on the yield stress $K_0 > 0$, where $\text{dev}(\boldsymbol{\sigma}) = \boldsymbol{\sigma} - (1/3)\text{trace}(\boldsymbol{\sigma})\mathbb{1}$ is the deviatoric part of the stress.

2.2. Perfect plasticity revisited

We start with the classical Prandtl–Reuss model:
find displacements

$$\mathbf{u}: \bar{\Omega} \times [0, T] \longrightarrow \mathbf{R}^3$$

symmetric stresses

$$\boldsymbol{\sigma}: \Omega \times [0, T] \longrightarrow \text{Sym}(3)$$

symmetric plastic strains

$$\boldsymbol{\varepsilon}_p: \Omega \times [0, T] \longrightarrow \text{Sym}(3)$$

and a plastic multiplier

$$\gamma: \Omega \times [0, T] \longrightarrow \mathbf{R}$$

satisfying the essential boundary conditions

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{u}_D(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Gamma_D \times [0, T]$$

the linear elastic constitutive relation

$$\boldsymbol{\sigma}(\mathbf{x}, t) = \mathbb{C}: (\boldsymbol{\varepsilon}(\mathbf{u})(\mathbf{x}, t) - \boldsymbol{\varepsilon}_p(\mathbf{x}, t)), \quad (\mathbf{x}, t) \in \Omega \times [0, T]$$

the equilibrium equations

$$-\operatorname{div} \boldsymbol{\sigma}(\mathbf{x}, t) = \mathbf{b}(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Omega \times [0, T] \quad (1a)$$

$$\boldsymbol{\sigma}(\mathbf{x}, t) \mathbf{n}(\mathbf{x}) = \mathbf{t}_N(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Gamma_N \times [0, T] \quad (1b)$$

the local flow rule

$$\dot{\boldsymbol{\varepsilon}}_p(\mathbf{x}, t) = \gamma(\mathbf{x}, t) \frac{\operatorname{dev}(\boldsymbol{\sigma}(\mathbf{x}, t))}{|\operatorname{dev}(\boldsymbol{\sigma}(\mathbf{x}, t))|}, \quad (\mathbf{x}, t) \in \Omega \times [0, T] \quad (2)$$

and the complementary conditions

$$\gamma(\mathbf{x}, t)(|\operatorname{dev}(\boldsymbol{\sigma}(\mathbf{x}, t))| - K_0) = 0, \quad \gamma(\mathbf{x}, t) \geq 0, \quad |\operatorname{dev}(\boldsymbol{\sigma}(\mathbf{x}, t))| \leq K_0 \quad (3)$$

The flow rule and complementary conditions can be reformulated in the form of a dissipation inequality, and the equilibrium equation can be given in an integrated form. To this end we define the spaces $\mathbf{S} = L_2(\Omega, \operatorname{Sym}(3))$, $\mathbf{E} = \{\boldsymbol{\eta} \in \mathbf{S} : \operatorname{trace}(\boldsymbol{\eta}) = 0\}$, $\mathbf{K} = \{\boldsymbol{\tau} \in \mathbf{S} : |\operatorname{dev}(\boldsymbol{\tau})| \leq K_0 \text{ a.e. in } \Omega\}$, and $\mathbf{V} = H^1(\Omega, \mathbf{R}^3)$, $\mathbf{V}_0 = \{\mathbf{v} \in \mathbf{V} : \mathbf{v}|_{\Gamma_D} = 0\}$, $\mathbf{V}(\mathbf{u}_D) = \{\mathbf{v} \in \mathbf{V} : \mathbf{v}|_{\Gamma_D} = \mathbf{u}_D\}$.

Lemma 1

If $\boldsymbol{\sigma}(t) \in \mathbf{K}$, then we have (the integrated dissipation inequality)

$$\int_{\Omega} K_0 |\delta \boldsymbol{\varepsilon}_p| \, d\mathbf{x} \geq \int_{\Omega} K_0 |\dot{\boldsymbol{\varepsilon}}_p(t)| \, d\mathbf{x} + \int_{\Omega} \boldsymbol{\sigma}(t) : (\delta \boldsymbol{\varepsilon}_p - \dot{\boldsymbol{\varepsilon}}_p(t)) \, d\mathbf{x}, \quad \delta \boldsymbol{\varepsilon}_p \in \mathbf{E} \quad (4)$$

Proof

The flow rule (2) gives $\gamma(t) = |\dot{\boldsymbol{\varepsilon}}_p(t)|$ and thus

$$\dot{\boldsymbol{\varepsilon}}_p(t) : \boldsymbol{\sigma}(t) = \gamma \frac{\operatorname{dev}(\boldsymbol{\sigma}(t)) : \boldsymbol{\sigma}(t)}{|\operatorname{dev}(\boldsymbol{\sigma}(t))|} = |\dot{\boldsymbol{\varepsilon}}_p(t)| |\operatorname{dev}(\boldsymbol{\sigma}(t))| = K_0 |\dot{\boldsymbol{\varepsilon}}_p(t)|$$

i.e. $0 = K_0 |\dot{\boldsymbol{\varepsilon}}_p(t)| - \boldsymbol{\sigma}(t) : \dot{\boldsymbol{\varepsilon}}_p(t)$. Together with

$$K_0 |\delta \boldsymbol{\varepsilon}_p| \geq |\operatorname{dev}(\boldsymbol{\sigma}(t))| |\delta \boldsymbol{\varepsilon}_p| \geq \operatorname{dev}(\boldsymbol{\sigma}(t)) : \delta \boldsymbol{\varepsilon}_p = \boldsymbol{\sigma}(t) : \delta \boldsymbol{\varepsilon}_p$$

and integrating in Ω this gives the result. $\square$

The equilibrium equation (1a) together with the dissipation inequality (4) gives

$$\begin{aligned} & \int_{\Omega} \boldsymbol{\sigma}(t) : \boldsymbol{\varepsilon}(\delta \mathbf{u}) \, d\mathbf{x} + \int_{\Omega} K_0 |\delta \boldsymbol{\varepsilon}_p| \, d\mathbf{x} \\ & \geq \ell(t, \delta \mathbf{u}) + \int_{\Omega} K_0 |\dot{\boldsymbol{\varepsilon}}_p(t)| \, d\mathbf{x} + \int_{\Omega} \boldsymbol{\sigma}(t) : (\delta \boldsymbol{\varepsilon}_p - \dot{\boldsymbol{\varepsilon}}_p(t)) \, d\mathbf{x} \end{aligned}$$

Substituting the constitutive relation $\boldsymbol{\sigma}(t) = \mathbb{C} : (\boldsymbol{\varepsilon}(\mathbf{u}(t)) - \boldsymbol{\varepsilon}_p(t))$ and testing with $\delta \mathbf{u} - \dot{\mathbf{u}}(t)$ yield

$$\begin{aligned} & \int_{\Omega} (\boldsymbol{\varepsilon}(\mathbf{u}(t)) - \boldsymbol{\varepsilon}_p(t)) : \mathbb{C} : \boldsymbol{\varepsilon}(\delta \mathbf{u} - \dot{\mathbf{u}}(t)) \, d\mathbf{x} + \int_{\Omega} K_0 |\delta \boldsymbol{\varepsilon}_p| \, d\mathbf{x} \\ & \geq \ell(t, \delta \mathbf{u} - \dot{\mathbf{u}}(t)) + \int_{\Omega} K_0 |\dot{\boldsymbol{\varepsilon}}_p(t)| \, d\mathbf{x} + \int_{\Omega} (\boldsymbol{\varepsilon}(\mathbf{u}(t)) - \boldsymbol{\varepsilon}_p(t)) : \mathbb{C} : (\delta \boldsymbol{\varepsilon}_p - \dot{\boldsymbol{\varepsilon}}_p(t)) \, d\mathbf{x} \end{aligned}$$

Defining the symmetric bilinear form

$$a_{pp}((\mathbf{u}, \boldsymbol{\varepsilon}_p), (\delta \mathbf{u}, \delta \boldsymbol{\varepsilon}_p)) = \int_{\Omega} (\boldsymbol{\varepsilon}(\mathbf{u}) - \boldsymbol{\varepsilon}_p) : \mathbb{C} : (\boldsymbol{\varepsilon}(\delta \mathbf{u}) - \delta \boldsymbol{\varepsilon}_p) \, d\mathbf{x}$$

(corresponding to perfect plasticity) and the convex, one-homogeneous integrated dissipation functional

$$j(\dot{\boldsymbol{\varepsilon}}_p) = \int_{\Omega} K_0 |\dot{\boldsymbol{\varepsilon}}_p| \, d\mathbf{x}$$

allows one to rewrite the equations of quasi-static infinitesimal plasticity as variational inequality:

$$a_{pp}((\mathbf{u}(t), \boldsymbol{\varepsilon}_p(t)), (\delta \mathbf{u}, \delta \boldsymbol{\varepsilon}_p) - (\dot{\mathbf{u}}(t), \dot{\boldsymbol{\varepsilon}}_p(t))) + j(\delta \boldsymbol{\varepsilon}_p) - j(\dot{\boldsymbol{\varepsilon}}_p(t)) \geq \ell(t, \delta \mathbf{u} - \dot{\mathbf{u}}(t))$$

2.3. Local kinematic hardening

Since $a_{pp}(\cdot, \cdot)$ is not coercive on $\mathbf{V}_0 \times \mathbf{E}$, we next study a regularized problem defining

$$a_{kh}((\mathbf{u}, \boldsymbol{\varepsilon}_p), (\delta \mathbf{u}, \delta \boldsymbol{\varepsilon}_p)) = \int_{\Omega} (\boldsymbol{\varepsilon}(\mathbf{u}) - \boldsymbol{\varepsilon}_p) : \mathbb{C} : (\boldsymbol{\varepsilon}(\delta \mathbf{u}) - \delta \boldsymbol{\varepsilon}_p) \, d\mathbf{x} + \int_{\Omega} \boldsymbol{\varepsilon}_p : \mathbb{D} : \delta \boldsymbol{\varepsilon}_p \, d\mathbf{x}$$

with a local kinematic hardening modulus $\mathbb{D} = \mu H_0 \text{id}$ (where $H_0 > 0$ is a nondimensional scaling factor).

For $c = 2/H_0 \geq 0$ we have $\boldsymbol{\varepsilon}_p : \mathbb{C} : \boldsymbol{\varepsilon}_p = 2\mu \boldsymbol{\varepsilon}_p : \boldsymbol{\varepsilon}_p = c \boldsymbol{\varepsilon}_p : \mathbb{D} : \boldsymbol{\varepsilon}_p$. This gives

$$(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_p) : \mathbb{C} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_p) + \boldsymbol{\varepsilon}_p : \mathbb{D} : \boldsymbol{\varepsilon}_p \geq \frac{1}{1+2c} \boldsymbol{\varepsilon} : \mathbb{C} : \boldsymbol{\varepsilon} + \frac{1}{2} \boldsymbol{\varepsilon}_p : \mathbb{D} : \boldsymbol{\varepsilon}_p$$

and therefore (by Korn's inequality)

$$a_{kh}((\mathbf{u}, \boldsymbol{\varepsilon}_p), (\mathbf{u}, \boldsymbol{\varepsilon}_p)) \geq C_1 \|(\boldsymbol{\varepsilon}(\mathbf{u}), \boldsymbol{\varepsilon}_p)\|_{L_2(\Omega)}^2 \geq C_2 \|(\mathbf{u}, \boldsymbol{\varepsilon}_p)\|_{\mathbf{V} \times \mathbf{E}}^2 \quad (5)$$

with $\|\mathbf{v}\|_{\mathbf{V}} = \|\mathbf{v}\|_{H^1(\Omega, \mathbf{R}^3)}$ and $\|\boldsymbol{\varepsilon}\|_{\mathbf{E}} = \|\boldsymbol{\varepsilon}\|_{L_2(\Omega, \mathbf{R}^{3 \times 3})}$. Now, the standard theory applies [32, Theorem 7.3]:

Theorem 2

A unique solution $(\mathbf{u}, \boldsymbol{\varepsilon}_p) \in H^1(0, T; \mathbf{V} \times \mathbf{E})$ with $\mathbf{u}(t) \in \mathbf{V}(\mathbf{u}_D)$ and

$$a_{kh}((\mathbf{u}(t), \boldsymbol{\varepsilon}_p(t)), (\delta \mathbf{u}, \delta \boldsymbol{\varepsilon}_p) - (\dot{\mathbf{u}}(t), \dot{\boldsymbol{\varepsilon}}_p(t))) + j(\delta \boldsymbol{\varepsilon}_p) - j(\dot{\boldsymbol{\varepsilon}}_p(t)) \geq \ell(t, \delta \mathbf{u} - \dot{\mathbf{u}}(t)) \quad (6)$$

exists for all $(\delta \mathbf{u}, \delta \boldsymbol{\varepsilon}_p) \in \mathbf{V}_0 \times \mathbf{E}$ and a.a. $t \in [0, T]$.

Testing with $\delta \mathbf{u} = \dot{\mathbf{u}}(t)$ in (6) and substituting the constitutive equation for the stress yield the dissipation inequality for plasticity with hardening in the form

$$\int_{\Omega} K_0 |\dot{\boldsymbol{\varepsilon}}_p| \, d\mathbf{x} \geq \int_{\Omega} K_0 |\dot{\boldsymbol{\varepsilon}}_p(t)| \, d\mathbf{x} + \int_{\Omega} (\boldsymbol{\sigma}(t) - \mathbb{D} : \boldsymbol{\varepsilon}_p(t)) : (\delta \boldsymbol{\varepsilon}_p - \dot{\boldsymbol{\varepsilon}}_p(t)) \, d\mathbf{x} \quad (7)$$

Within the hardening model, $\boldsymbol{\beta} = \mathbb{D} : \boldsymbol{\varepsilon}_p$ is the local symmetric backstress, and $\boldsymbol{\alpha} = \boldsymbol{\sigma} - \boldsymbol{\beta} = \boldsymbol{\sigma} - \mathbb{D} : \boldsymbol{\varepsilon}_p$ is the automatically symmetric relative (elastic) stress (cf. [33, Chapter 3.3.1]).

Lemma 3

If (7) holds for all $\delta \varepsilon_p \in \mathbf{E}$, we have $\alpha(t) \in \mathbf{K}$ a.e. in Ω . In addition, it holds that $\dot{\varepsilon}_p(t) = \mathbf{0}$ a.e. in the elastic zone $\Omega_{el}(t) = \{\mathbf{x} \in \Omega : |\text{dev} \alpha(t)| < K_0 \text{ a.e. in some neighborhood of } \mathbf{x}\}$, and we have $K_0 \varepsilon_p(t) = |\varepsilon_p(t)| \text{dev}(\alpha(t))$ a.e. in Ω .

Proof

Testing (7) with $s \delta \varepsilon_p$ for $s > 0$ and then dividing by s give

$$\int_{\Omega} K_0 |\delta \varepsilon_p| \, d\mathbf{x} \geq \frac{1}{s} \int_{\Omega} K_0 |\dot{\varepsilon}_p(t)| \, d\mathbf{x} + \int_{\Omega} \alpha(t) : \delta \varepsilon_p \, d\mathbf{x} - \frac{1}{s} \int_{\Omega} \alpha(t) : \dot{\varepsilon}_p(t) \, d\mathbf{x}$$

Passing to the limit $s \rightarrow \infty$ yields

$$\int_{\Omega} \text{dev}(\alpha(t)) : \delta \varepsilon_p \, d\mathbf{x} = \int_{\Omega} \alpha(t) : \delta \varepsilon_p \, d\mathbf{x} \leq \int_{\Omega} K_0 |\delta \varepsilon_p| \, d\mathbf{x} \quad (8)$$

for all $\delta \varepsilon_p \in \mathbf{E}$. For all open subsets $\tilde{\Omega} \subset \Omega$ we can substitute a test function $\delta \varepsilon_p$, which is defined as $\delta \varepsilon_p(\mathbf{x}) = \text{dev}(\alpha(\mathbf{x}, t))$ for $\mathbf{x} \in \tilde{\Omega}$ and $\delta \varepsilon_p(\mathbf{x}) = \mathbf{0}$ else. This results in

$$\int_{\tilde{\Omega}} |\text{dev}(\alpha(t))|^2 \, d\mathbf{x} \leq \int_{\tilde{\Omega}} K_0 |\text{dev}(\alpha(t))| \, d\mathbf{x}$$

Since $\tilde{\Omega} \subset \Omega$ is arbitrary, this gives $|\text{dev}(\alpha(t))|^2 \leq K_0 |\text{dev}(\alpha(t))|$ a.e. in Ω , i.e. $\text{dev}(\alpha(t)) \in \mathbf{K}$. Now, testing (7) with $\delta \varepsilon_p = s \dot{\varepsilon}_p(t)$ on $\tilde{\Omega} \subset \Omega$ gives for $s > 0$

$$(s-1) \int_{\tilde{\Omega}} K_0 |\dot{\varepsilon}_p(t)| \, d\mathbf{x} \geq (s-1) \int_{\tilde{\Omega}} \alpha(t) : \dot{\varepsilon}_p(t) \, d\mathbf{x}$$

and thus (by substituting $s = 1 \pm \frac{1}{2}$) equality

$$\int_{\tilde{\Omega}} K_0 |\dot{\varepsilon}_p(t)| \, d\mathbf{x} = \int_{\tilde{\Omega}} \alpha(t) : \dot{\varepsilon}_p(t) \, d\mathbf{x} = \int_{\tilde{\Omega}} \text{dev}(\alpha(t)) : \dot{\varepsilon}_p(t) \, d\mathbf{x}$$

Then, $|\text{dev}(\alpha(t))| \leq K_0$ yields $K_0 |\dot{\varepsilon}_p(t)| = \alpha(t) : \dot{\varepsilon}_p(t)$ a.e. in Ω . In the case of $|\alpha(\mathbf{x}, t)| < K_0$, this implies that $\dot{\varepsilon}_p(\mathbf{x}, t) = \mathbf{0}$; otherwise we have the equality in the Cauchy–Schwarz inequality. Thus, $s \text{dev}(\alpha(\mathbf{x}, t)) = \dot{\varepsilon}_p(\mathbf{x}, t)$ are linearly dependent with $s = |\dot{\varepsilon}_p(\mathbf{x}, t)| / K_0$. $\square$

Reformulating this lemma shows that the solution $(\mathbf{u}, \varepsilon_p)$ of (6) satisfies the point-wise flow rule

$$\dot{\varepsilon}_p = \gamma \frac{\text{dev}(\alpha)}{|\text{dev}(\alpha)|}, \quad \gamma = |\dot{\varepsilon}_p|, \quad \sigma = \mathbb{C} : (\varepsilon(\mathbf{u}) - \varepsilon_p), \quad \alpha = \sigma - \mathbb{D} : \varepsilon_p \quad (9)$$

and the complementary conditions

$$\gamma(|\text{dev}(\alpha)| - K_0) = 0, \quad \gamma \geq 0, \quad |\text{dev}(\alpha)| \leq K_0 \quad (10)$$

a.e. in $\Omega \times [0, T]$ which can also be reformulated as a subdifferential inclusion [20, p. 17].

Remark 4

The equivalence of (point-wise) flow rules and (integrated) dissipation inequalities is well studied in the general framework of convex analysis [32, Chapter 4; 34]. Extensions of this concept are

considered within the energetic plasticity approach by Mielke [35]. In general, corresponding equivalence relations hold for local models only [20].

2.4. Nonlocal-dislocation-based plasticity with symmetric plastic strains

Next, we extend $a_{\text{kh}}(\cdot, \cdot)$ by a further term involving nonlocal dislocation density effects to read

$$a_{\text{nl}}((\mathbf{u}, \boldsymbol{\varepsilon}_{\text{p}}), (\delta \mathbf{u}, \delta \boldsymbol{\varepsilon}_{\text{p}})) = a_{\text{kh}}((\mathbf{u}, \boldsymbol{\varepsilon}_{\text{p}}), (\delta \mathbf{u}, \delta \boldsymbol{\varepsilon}_{\text{p}})) + \int_{\Omega} \text{curl}(\boldsymbol{\varepsilon}_{\text{p}}) : \mathbb{E} : \text{curl}(\delta \boldsymbol{\varepsilon}_{\text{p}}) \, \text{d}\mathbf{x}$$

with $\mathbb{E} = \mu L_c^2 \text{id}$. Here, $L_c > 0$ is the internal plastic length scale with units of length. The curl-related term represents the energy stored in the material due to deformation incompatibility. In particular, diffuse phase boundaries are energetically favored by larger values of L_c , while sharp phase boundaries are favored by smaller values of L_c . In the next theorem we will show that this extension of the bilinear form is equivalent to modifying the flow rule (9) to (14) by appending a curlcurl-term.

We define the space

$$\mathbf{E}_{\text{nl}} := \{\boldsymbol{\varepsilon}_{\text{p}} \in L_2(\Omega, \mathbf{R}^{d,d}) : \text{curl}(\boldsymbol{\varepsilon}_{\text{p}}) \in L_2(\Omega, \mathbf{R}^{d,d}), \text{trace}(\boldsymbol{\varepsilon}_{\text{p}}) = 0, \text{skew}(\boldsymbol{\varepsilon}_{\text{p}}) = 0\}$$

(where the curl-operator is applied row-wise on $\boldsymbol{\varepsilon}_{\text{p}}$). Equipped with the norm

$$\|\boldsymbol{\varepsilon}_{\text{p}}\|_{\mathbf{E}_{\text{nl}}}^2 := \|\boldsymbol{\varepsilon}_{\text{p}}\|_{L_2(\Omega, \mathbf{R}^{d,d})}^2 + \|\text{curl} \boldsymbol{\varepsilon}_{\text{p}}\|_{L_2(\Omega, \mathbf{R}^{d,d})}^2 \quad (11)$$

this is a closed subspace of $H(\text{curl}, \Omega)^3$. From (5) we conclude that $a_{\text{nl}}(\cdot, \cdot)$ is elliptic in $\mathbf{V}_0 \times \mathbf{E}_{\text{nl}}$, so that again [32, Theorem 7.3] applies and gives the following:

Theorem 5

A unique solution $(\mathbf{u}, \boldsymbol{\varepsilon}_{\text{p}}) \in H^1(0, T; \mathbf{V} \times \mathbf{E}_{\text{nl}})$ with $\mathbf{u}(t) \in \mathbf{V}(\mathbf{u}_{\text{D}})$ and

$$a_{\text{nl}}((\mathbf{u}(t), \boldsymbol{\varepsilon}_{\text{p}}(t)), (\delta \mathbf{u}, \delta \boldsymbol{\varepsilon}_{\text{p}}) - (\dot{\mathbf{u}}(t), \dot{\boldsymbol{\varepsilon}}_{\text{p}}(t))) + j(\delta \boldsymbol{\varepsilon}_{\text{p}}) - j(\dot{\boldsymbol{\varepsilon}}_{\text{p}}(t)) \geq \ell(t, \delta \mathbf{u} - \dot{\mathbf{u}}(t)) \quad (12)$$

for all $(\delta \mathbf{u}, \delta \boldsymbol{\varepsilon}_{\text{p}}) \in \mathbf{V}_0 \times \mathbf{E}_{\text{nl}}$ and a.a. $t \in [0, T]$ exists.

Testing with $\delta \mathbf{u} = \dot{\mathbf{u}}(t)$ in (12) and substituting the stress $\boldsymbol{\sigma} = \mathbb{C} : (\boldsymbol{\varepsilon}(\mathbf{u}) - \boldsymbol{\varepsilon}_{\text{p}})$ yield the corresponding integrated dissipation inequality for the nonlocal plasticity model in the form

$$\begin{aligned} \int_{\Omega} K_0 |\delta \boldsymbol{\varepsilon}_{\text{p}}| \, \text{d}\mathbf{x} &\geq \int_{\Omega} K_0 |\dot{\boldsymbol{\varepsilon}}_{\text{p}}(t)| \, \text{d}\mathbf{x} + \int_{\Omega} (\boldsymbol{\sigma}(t) - \mathbb{D} : \boldsymbol{\varepsilon}_{\text{p}}(t)) : (\delta \boldsymbol{\varepsilon}_{\text{p}} - \dot{\boldsymbol{\varepsilon}}_{\text{p}}(t)) \, \text{d}\mathbf{x} \\ &\quad - \int_{\Omega} \text{curl}(\boldsymbol{\varepsilon}_{\text{p}}(t)) : \mathbb{E} : \text{curl}(\delta \boldsymbol{\varepsilon}_{\text{p}} - \dot{\boldsymbol{\varepsilon}}_{\text{p}}(t)) \, \text{d}\mathbf{x} \end{aligned} \quad (13)$$

Without additional regularity, we cannot derive a point-wise flow rule in this case (in general, the stress is not bounded in L_{∞}). Formally, if $\text{curl}(\mathbb{E} : \text{curl}(\boldsymbol{\varepsilon}_{\text{p}}(t)))$ exists and if one includes homogeneous boundary conditions in $\mathbf{E}_{\text{nl}}$, integration by parts yields the dissipation inequality in a strong form

$$\int_{\Omega} K_0 |\delta \boldsymbol{\varepsilon}_{\text{p}}| \, \text{d}\mathbf{x} \geq \int_{\Omega} K_0 |\dot{\boldsymbol{\varepsilon}}_{\text{p}}(t)| \, \text{d}\mathbf{x} + \int_{\Omega} (\boldsymbol{\sigma}(t) - \mathbb{D} : \boldsymbol{\varepsilon}_{\text{p}}(t) - \text{curl}(\mathbb{E} : \text{curl}(\boldsymbol{\varepsilon}_{\text{p}}(t)))) : (\delta \boldsymbol{\varepsilon}_{\text{p}} - \dot{\boldsymbol{\varepsilon}}_{\text{p}}(t)) \, \text{d}\mathbf{x}$$

This corresponds to flow rule (9) and complementarity conditions (10), where the relative stress has the form $\boldsymbol{\sigma} - \mathbb{D} : \boldsymbol{\varepsilon}_p - \text{curl}(\mathbb{E} : \text{curl}(\boldsymbol{\varepsilon}_p))$. In fact, since $\boldsymbol{\varepsilon}_p$ is symmetric, only its symmetric part enters the model. Thus, for simplicity of notation, we denote in what follows the symmetrized relative stress by $\boldsymbol{\alpha}$. This means that with the preceding provisions, a smooth solution $(\mathbf{u}, \boldsymbol{\varepsilon}_p)$ of (12) satisfies the point-wise flow rule

$$\dot{\boldsymbol{\varepsilon}}_p = \gamma \frac{\text{dev}(\boldsymbol{\alpha})}{|\text{dev}(\boldsymbol{\alpha})|}, \quad \gamma = |\dot{\boldsymbol{\varepsilon}}_p|, \quad \boldsymbol{\alpha} = \boldsymbol{\sigma} - \mathbb{D} : \boldsymbol{\varepsilon}_p - \text{sym}(\text{curl}(\mathbb{E} : \text{curl}(\boldsymbol{\varepsilon}_p))) \quad (14)$$

and the complementary conditions

$$\gamma(|\text{dev}(\text{sym} \boldsymbol{\alpha})| - K_0) = 0, \quad \gamma \geq 0, \quad |\text{dev}(\text{sym} \boldsymbol{\alpha})| \leq K_0 \quad (15)$$

a.e. in $\Omega \times [0, T]$. In Theorem 8 this is addressed in more detail, where a saddle point formulation is introduced in order to provide an elegant framework, which avoids extra boundary conditions and which recovers (numerically) a point-wise flow rule.

Remark 6

This construction of a nonlocal model is only one prototype for a large class of dislocation models, which can be handled in the same framework. Observe that our model can be obtained as a special nonspin case of a model in [20]. Since our main focus is the clear presentation of a numerical solution method, we do not discuss other models; see [15, 20, 36] for other proposals in this respect.

3. INCREMENTAL NONLOCAL PLASTICITY

Replacing the time derivative by backward difference quotients and introducing suitable finite element spaces for displacements and plastic strains directly yield the discrete analog to the nonlocal problem (12). This incremental problem is fully implicit, and the solution of the incremental problem can be characterized by a minimization problem.

Unfortunately, this approach is not compatible with standard (local) plasticity, since it requires discrete plastic strains in $H(\text{curl})$. Thus, in the second step we discuss a saddle point formulation (introducing an additional variable for the approximation of $\text{curl} \boldsymbol{\varepsilon}_p$), which results in a constrained minimization problem.

3.1. A primal approach

Let $\mathbf{V}^h \subset \mathbf{V}$ be a finite element discretization of the displacements, and let $0 = t_0 < t_1 < \dots < t_N = T$ be a decomposition of the time interval $[0, T]$. We set $\Delta \mathbf{u}_D^n = \mathbf{u}_D(t_n) - \mathbf{u}_D(t_{n-1})$, $\mathbf{V}^h(\mathbf{u}_D) = \{\mathbf{v}^h : \mathbf{v}_h(\mathbf{x}) = \mathbf{u}_D(\mathbf{x}) \text{ for all nodal points on } \Gamma_D\}$ and $\mathbf{V}_0^h = \mathbf{V}^h(\mathbf{0})$. Let $\mathbf{E}_{nl}^h \subset \mathbf{E}_{nl}$ be a finite element discretization for the plastic strains. Note that this requires $H(\text{curl})$ -conforming finite elements in $\mathbf{E}_{nl}^h$, whereas in the classical setting $\mathbf{E}$ can be approximated simply by Gauss point values. In our applications, we use standard H^1 -conforming finite elements $\mathbf{V}^h$ and Ned  lec elements in $H(\text{curl})$ [37].

For fixed t_n and given $(\mathbf{u}^{h,n-1}, \boldsymbol{\varepsilon}_p^{h,n-1}) \in \mathbf{V}^h \times \mathbf{E}_{nl}^h$ we define

$$\ell_n(\delta \mathbf{u}^h) = \ell(t_n, \delta \mathbf{u}^h), \quad \ell_{nl}^{h,n}(\delta \mathbf{u}^h, \delta \boldsymbol{\varepsilon}_p^h) = \ell_n(\delta \mathbf{u}^h) - a_{nl}((\mathbf{u}^{h,n-1}, \boldsymbol{\varepsilon}_p^{h,n-1}), (\delta \mathbf{u}^h, \delta \boldsymbol{\varepsilon}_p^h))$$

Now we obtain by Han and Reddy [32, Theorem 6.6] for the backward Euler discretization of (12):

Theorem 7

A unique minimizer $(\Delta \mathbf{u}^{h,n}, \Delta \boldsymbol{\varepsilon}_p^{h,n}) \in \mathbf{V}^h(\Delta \mathbf{u}_D^n) \times \mathbf{E}_{nl}^h$ of

$$J_{nl}^{h,n}(\Delta \mathbf{u}^h, \Delta \boldsymbol{\varepsilon}_p^h) = \frac{1}{2} a_{nl}((\Delta \mathbf{u}^h, \Delta \boldsymbol{\varepsilon}_p^h), (\Delta \mathbf{u}^h, \Delta \boldsymbol{\varepsilon}_p^h)) + j(\Delta \boldsymbol{\varepsilon}_p^h) - \ell_{nl}^{h,n}(\Delta \mathbf{u}^h, \Delta \boldsymbol{\varepsilon}_p^h) \quad (16)$$

exists. Moreover, the minimizer is characterized by the discrete variational inequality

$$\begin{aligned} a_{nl}((\mathbf{u}^{h,n-1} + \Delta \mathbf{u}^{h,n}, \boldsymbol{\varepsilon}_p^{h,n-1} + \Delta \boldsymbol{\varepsilon}_p^{h,n}), (\delta \mathbf{u}^h, \delta \boldsymbol{\varepsilon}_p^n) - (\Delta \mathbf{u}^{h,n}, \Delta \boldsymbol{\varepsilon}_p^{h,n})) \\ + j(\delta \boldsymbol{\varepsilon}_p^h) - j(\Delta \boldsymbol{\varepsilon}_p^{h,n}) \geq \ell_n(\delta \mathbf{u}^h - \Delta \mathbf{u}^{h,n}), \quad (\delta \mathbf{u}^h, \delta \boldsymbol{\varepsilon}_p^h) \in \mathbf{V}_0^h \times \mathbf{E}_{nl}^h \end{aligned} \quad (17)$$

Thus, the incremental problem is well defined, and we set

$$(\mathbf{u}^{h,n}, \boldsymbol{\varepsilon}_p^{h,n}) = (\mathbf{u}^{h,n-1}, \boldsymbol{\varepsilon}_p^{h,n-1}) + (\Delta \mathbf{u}^{h,n}, \Delta \boldsymbol{\varepsilon}_p^{h,n}) \quad (18)$$

3.2. A mixed formulation

There is no need to impose or discuss explicit boundary conditions on $\boldsymbol{\varepsilon}_p$, since coercivity is automatically satisfied. This results in natural boundary conditions for the variational solution. In the dual formulation this requires essential boundary conditions for the dual test functions: for given $\boldsymbol{\varepsilon}_p \in H(\text{curl}, \Omega)^3$ we can define $\mathbf{g}_p \in H_0(\text{curl}, \Omega)^3 = \{\mathbf{g} \in H(\text{curl}, \Omega)^3 : \mathbf{g} \times \mathbf{n} = \mathbf{0}\}$ by

$$\int_{\Omega} \mathbf{g}_p : \mathbb{E}^{-1} : \delta \mathbf{g}_p \, d\mathbf{x} = \int_{\Omega} \boldsymbol{\varepsilon}_p : \text{curl}(\delta \mathbf{g}_p) \, d\mathbf{x}, \quad \delta \mathbf{g}_p \in H_0(\text{curl}, \Omega)^3$$

which defines $\mathbf{g}_p = \mathbb{E} : \text{curl}(\boldsymbol{\varepsilon}_p)$ in terms of distributions.

Thus, in order to obtain a discrete flow rule for the nonlocal model, we consider a mixed formulation in $\mathbf{E}^h \times \mathbf{G}^h \subset \mathbf{E} \times H_0(\text{curl}, \Omega)^3$: we introduce a finite element function $\mathbf{g}_p^h \in \mathbf{G}^h$ approximating $\mathbb{E} : \text{curl}(\boldsymbol{\varepsilon}_p^h)$ in a variational (weak) sense: the pair $(\mathbf{g}_p^h, \boldsymbol{\varepsilon}_p^h) \in \mathbf{G}^h \times \mathbf{E}^h$ is assumed to be coupled by

$$\int_{\Omega} \mathbf{g}_p^h : \mathbb{E}^{-1} : \delta \mathbf{g}_p^h \, d\mathbf{x} = \int_{\Omega} \boldsymbol{\varepsilon}_p^h : \text{curl}(\delta \mathbf{g}_p^h) \, d\mathbf{x}, \quad \delta \mathbf{g}_p^h \in \mathbf{G}^h \quad (19)$$

The extended bilinear form is obtained from $a_{nl}(\cdot, \cdot)$ by replacing $\mathbb{E} : \text{curl}(\boldsymbol{\varepsilon}_p)$ with $\mathbf{g}_p$, i.e.

$$a_{mx}((\mathbf{u}, \boldsymbol{\varepsilon}_p, \mathbf{g}_p), (\delta \mathbf{u}, \delta \boldsymbol{\varepsilon}_p, \delta \mathbf{g}_p)) = a_{kh}((\mathbf{u}, \boldsymbol{\varepsilon}_p), (\delta \mathbf{u}, \delta \boldsymbol{\varepsilon}_p)) + \int_{\Omega} \mathbf{g}_p : \mathbb{E}^{-1} : \delta \mathbf{g}_p \, d\mathbf{x}$$

The bilinear form $a_{mx}(\cdot, \cdot)$ is positive definite in the discrete, extended space $\mathbf{V}_0^h \times \mathbf{E}^h \times \mathbf{G}^h$ and thus in the closed subspace $\mathbf{X}^h(\mathbf{0})$, where

$$\mathbf{X}^h(\mathbf{u}_D) = \{(\mathbf{u}^h, \boldsymbol{\varepsilon}_p^h, \mathbf{g}_p^h) \in \mathbf{V}^h(\mathbf{u}_D) \times \mathbf{E}^h \times \mathbf{G}^h : (\mathbf{g}_p^h, \boldsymbol{\varepsilon}_p^h) \text{ satisfies (19)}\}$$

For the incremental problem we now fix the values $(\mathbf{u}^{h,n-1}, \boldsymbol{\varepsilon}_p^{h,n-1}, \mathbf{g}_p^{h,n-1}) \in \mathbf{X}^h(\mathbf{u}_D^{n-1})$ of the previous time step. Introducing

$$\ell_{mx}^{h,n}(\delta \mathbf{u}^h, \delta \boldsymbol{\varepsilon}_p^h, \delta \mathbf{g}_p^h) = \ell_n(\delta \mathbf{u}^h) - a_{mx}((\mathbf{u}^{h,n-1}, \boldsymbol{\varepsilon}_p^{h,n-1}, \mathbf{g}_p^{h,n-1}), (\delta \mathbf{u}^h, \delta \boldsymbol{\varepsilon}_p^h, \delta \mathbf{g}_p^h)) \quad (20)$$

we obtain the following:

Theorem 8

A unique minimizer $(\Delta \mathbf{u}^{h,n}, \Delta \boldsymbol{\varepsilon}_p^{h,n}, \Delta \mathbf{g}_p^{h,n}) \in \mathbf{X}^h(\Delta \mathbf{u}_D^n)$ of

$$J_{\text{mx}}^{h,n}(\Delta \mathbf{u}^h, \Delta \boldsymbol{\varepsilon}_p^h, \Delta \mathbf{g}_p^h) = \frac{1}{2} a_{\text{mx}}((\Delta \mathbf{u}^h, \Delta \boldsymbol{\varepsilon}_p^h, \Delta \mathbf{g}_p^h), (\Delta \mathbf{u}^h, \Delta \boldsymbol{\varepsilon}_p^h, \Delta \mathbf{g}_p^h)) \\ + j(\Delta \boldsymbol{\varepsilon}_p^h) - \ell_{\text{mx}}^{h,n}(\Delta \mathbf{u}^h, \Delta \boldsymbol{\varepsilon}_p^h, \Delta \mathbf{g}_p^h)$$

exists. Moreover, $(\mathbf{u}^{h,n}, \boldsymbol{\varepsilon}_p^{h,n}, \mathbf{g}_p^{h,n}) = (\mathbf{u}^{h,n-1}, \boldsymbol{\varepsilon}_p^{h,n-1}, \mathbf{g}_p^{h,n-1}) + (\Delta \mathbf{u}^{h,n}, \Delta \boldsymbol{\varepsilon}_p^{h,n}, \Delta \mathbf{g}_p^{h,n})$ is characterized by the linear variational saddle point problem

$$\int_{\Omega} \boldsymbol{\sigma}^{h,n} : \mathbb{C} : \boldsymbol{\varepsilon}(\delta \mathbf{u}^h) \, d\mathbf{x} = \ell_n(\delta \mathbf{u}^h), \quad \delta \mathbf{u}^h \in \mathbf{V}_0^h \quad (21a)$$

$$\int_{\Omega} \mathbf{g}_p^{h,n} : \mathbb{E}^{-1} : \delta \mathbf{g}_p^h \, d\mathbf{x} = \int_{\Omega} \boldsymbol{\varepsilon}_p^{h,n} : \text{curl}(\delta \mathbf{g}_p^h) \, d\mathbf{x}, \quad \delta \mathbf{g}_p^h \in \mathbf{G}^h \quad (21b)$$

and the variational inequality

$$\int_{\Omega} K_0 |\delta \boldsymbol{\varepsilon}_p^h| \, d\mathbf{x} \geq \int_{\Omega} K_0 |\Delta \boldsymbol{\varepsilon}_p^{h,n}| \, d\mathbf{x} + \int_{\Omega} \boldsymbol{\alpha}^{h,n} : (\delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{h,n}) \, d\mathbf{x}, \quad \delta \boldsymbol{\varepsilon}_p^h \in \mathbf{E}^h \quad (21c)$$

with $\boldsymbol{\sigma}^{h,n} = \boldsymbol{\varepsilon}(\mathbf{u}^{h,n}) - \boldsymbol{\varepsilon}_p^{h,n}$ and $\boldsymbol{\alpha}^{h,n} = \boldsymbol{\sigma}^{h,n} - \mathbb{D} : \boldsymbol{\varepsilon}_p^{h,n} - \text{sym}(\text{curl}(\mathbf{g}_p^{h,n}))$.

Proof

The proof uses standard techniques of convex analysis and is included for convenience of the reader. Since $J_{\text{mx}}^{h,n}(\cdot)$ is uniformly convex, a unique minimizer $(\Delta \mathbf{u}^{h,n}, \Delta \boldsymbol{\varepsilon}_p^{h,n}, \Delta \mathbf{g}_p^{h,n})$ in the discrete space $\mathbf{X}^h(\Delta \mathbf{u}_D^n)$ exists. Now we show (21c). Therefore, we define

$$J_{\text{red}}^{h,n}(\delta \boldsymbol{\varepsilon}_p^h, \delta \mathbf{g}_p^h) = \frac{1}{2} a_{\text{mx}}((\Delta \mathbf{u}^{h,n}, \delta \boldsymbol{\varepsilon}_p^h, \delta \mathbf{g}_p^h), (\Delta \mathbf{u}^{h,n}, \delta \boldsymbol{\varepsilon}_p^h, \delta \mathbf{g}_p^h)), \quad (\delta \boldsymbol{\varepsilon}_p^h, \delta \mathbf{g}_p^h) \in \mathbf{E}^h \times \mathbf{G}^h$$

For any $s \in (0, 1)$, the inequality

$$J_{\text{mx}}^{h,n}(\Delta \mathbf{u}^{h,n}, \Delta \boldsymbol{\varepsilon}_p^{h,n}, \Delta \mathbf{g}_p^{h,n}) \leq J_{\text{mx}}^{h,n}(\Delta \mathbf{u}^{h,n}, \Delta \boldsymbol{\varepsilon}_p^{h,n} + s(\delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{h,n}), \Delta \mathbf{g}_p^{h,n} + s(\delta \mathbf{g}_p^h - \Delta \mathbf{g}_p^{h,n}))$$

can be rewritten as

$$J_{\text{red}}^{h,n}(\Delta \boldsymbol{\varepsilon}_p^{h,n}, \Delta \mathbf{g}_p^{h,n}) + j(\Delta \boldsymbol{\varepsilon}_p^{h,n}) \leq J_{\text{red}}^{h,n}(\Delta \boldsymbol{\varepsilon}_p^{h,n} + s(\delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{h,n}), \Delta \mathbf{g}_p^{h,n} + s(\delta \mathbf{g}_p^h - \Delta \mathbf{g}_p^{h,n})) \\ + j(\Delta \boldsymbol{\varepsilon}_p^{h,n} + s(\delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{h,n})) - s \ell_{\text{mx}}^{h,n}(\mathbf{0}, \delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{h,n})$$

Using the convexity of $j(\cdot)$, i.e.

$$j(\Delta \boldsymbol{\varepsilon}_p^{h,n} + s(\delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{h,n})) = j((1-s)\Delta \boldsymbol{\varepsilon}_p^{h,n} + s\delta \boldsymbol{\varepsilon}_p^h) \leq (1-s)j(\Delta \boldsymbol{\varepsilon}_p^{h,n}) + sj(\delta \boldsymbol{\varepsilon}_p^h)$$

gives

$$J_{\text{red}}^{h,n}(\Delta \boldsymbol{\varepsilon}_p^{h,n}, \Delta \mathbf{g}_p^{h,n}) \leq J_{\text{red}}^{h,n}(\Delta \boldsymbol{\varepsilon}_p^{h,n} + s(\delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{h,n}), \Delta \mathbf{g}_p^{h,n} + s(\delta \mathbf{g}_p^h - \Delta \mathbf{g}_p^{h,n})) \\ + s(j(\delta \boldsymbol{\varepsilon}_p^h) - j(\Delta \boldsymbol{\varepsilon}_p^{h,n})) - s \ell_{\text{mx}}^{h,n}(\mathbf{0}, \delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{h,n})$$

and thus

$$\begin{aligned} 0 &\leq s a_{\max}((\Delta \mathbf{u}^{h,n}, \Delta \boldsymbol{\varepsilon}_p^{h,n}, \Delta \mathbf{g}_p^{h,n}), (\mathbf{0}, \delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{n,h}, \delta \mathbf{g}_p^h - \Delta \mathbf{g}_p^{h,n})) \\ &\quad + s^2 a_{\max}((\mathbf{0}, \delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{n,h}, \delta \mathbf{g}_p^h - \Delta \mathbf{g}_p^{h,n}), (\mathbf{0}, \delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{n,h}, \delta \mathbf{g}_p^h - \Delta \mathbf{g}_p^{h,n})) \\ &\quad + s(j(\delta \boldsymbol{\varepsilon}_p^h) - j(\Delta \boldsymbol{\varepsilon}_p^{h,n})) - s \ell_{\max}^{h,n}(\mathbf{0}, \delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{h,n}) \end{aligned}$$

Dividing by s and then taking the limit $s \rightarrow 0$ yield

$$\begin{aligned} 0 &\leq a_{\max}((\Delta \mathbf{u}^{h,n}, \Delta \boldsymbol{\varepsilon}_p^{h,n}, \Delta \mathbf{g}_p^{h,n}), (\mathbf{0}, \delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{n,h}, \delta \mathbf{g}_p^h - \Delta \mathbf{g}_p^{h,n})) \\ &\quad + j(\delta \boldsymbol{\varepsilon}_p^h) - j(\Delta \boldsymbol{\varepsilon}_p^{h,n}) - \ell_{\max}^{h,n}(\mathbf{0}, \delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{h,n}) \end{aligned}$$

i.e.

$$\begin{aligned} j(\Delta \boldsymbol{\varepsilon}_p^{h,n}) &\leq - \int_{\Omega} \Delta \boldsymbol{\sigma}^{h,n} : (\delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{n,h}) \, d\mathbf{x} + \int_{\Omega} \Delta \boldsymbol{\varepsilon}_p^{h,n} : \mathbb{D} : (\delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{n,h}) \, d\mathbf{x} \\ &\quad + \int_{\Omega} \Delta \mathbf{g}_p^{h,n} : \mathbb{E}^{-1} : (\delta \mathbf{g}_p^h - \Delta \mathbf{g}_p^{h,n}) \, d\mathbf{x} + j(\delta \boldsymbol{\varepsilon}_p^h) \\ &\quad - \int_{\Omega} \boldsymbol{\sigma}^{h,n-1} : (\delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{n,h}) \, d\mathbf{x} + \int_{\Omega} \boldsymbol{\varepsilon}_p^{h,n-1} : \mathbb{D} : (\delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{n,h}) \, d\mathbf{x} \\ &\quad + \int_{\Omega} \mathbf{g}_p^{h,n-1} : \mathbb{E}^{-1} : (\delta \mathbf{g}_p^h - \Delta \mathbf{g}_p^{h,n}) \, d\mathbf{x} \end{aligned}$$

The linear constraint (19)

$$\int_{\Omega} (\delta \mathbf{g}_p^h - \Delta \mathbf{g}_p^{h,n}) : \mathbb{E}^{-1} : \mathbf{g}_p^{h,n} \, d\mathbf{x} = \int_{\Omega} (\delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{h,n}) : \text{curl}(\mathbf{g}_p^{h,n}) \, d\mathbf{x}$$

gives

$$\begin{aligned} j(\Delta \boldsymbol{\varepsilon}_p^{h,n}) &\leq - \int_{\Omega} \boldsymbol{\sigma}^{h,n} : (\delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{n,h}) \, d\mathbf{x} + \int_{\Omega} \boldsymbol{\varepsilon}_p^{h,n} : \mathbb{D} : (\delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{n,h}) \, d\mathbf{x} \\ &\quad + \int_{\Omega} \text{curl}(\mathbf{g}_p^{h,n}) : (\delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{h,n}) \, d\mathbf{x} + j(\delta \boldsymbol{\varepsilon}_p^h) \end{aligned}$$

which shows the dissipation inequality (21c).

Next, we derive (21a). Since the corresponding reduced functional

$$J_{\mathbf{u}}^{h,n}(\Delta \mathbf{u}^h) = J_{\max}^{h,n}(\Delta \mathbf{u}^h, \Delta \boldsymbol{\varepsilon}_p^{h,n}, \Delta \mathbf{g}_p^{h,n}), \quad \Delta \mathbf{u}^h \in \mathbf{V}^h(\Delta \mathbf{u}_D^n)$$

is quadratic with respect to $\Delta \mathbf{u}^h$, the minimizer $\Delta \mathbf{u}^{h,n}$ of $J_{\mathbf{u}}^{h,n}(\cdot)$ is a critical point of $J_{\mathbf{u}}^{h,n}(\cdot)$ and characterized by $DJ_{\mathbf{u}}^{h,n}(\Delta \mathbf{u}^{h,n})[(\delta \mathbf{u}^h)] = 0$, i.e.

$$a_{\max}((\Delta \mathbf{u}^{h,n}, \Delta \boldsymbol{\varepsilon}_p^{h,n}, \Delta \mathbf{g}_p^{h,n}), (\delta \mathbf{u}^h, \mathbf{0}, \mathbf{0})) - \ell_{\max}^{h,n}(\delta \mathbf{u}^h, \mathbf{0}, \mathbf{0}) = 0, \quad \delta \mathbf{u}^h \in \mathbf{V}_0^h$$

This yields for the stress increment $\Delta \boldsymbol{\sigma}^{h,n} = \mathbb{C} : (\boldsymbol{\varepsilon}(\Delta \mathbf{u}^{h,n}) - \Delta \boldsymbol{\varepsilon}_p^{h,n})$

$$\int_{\Omega} \Delta \boldsymbol{\sigma}^{h,n} : \boldsymbol{\varepsilon}(\delta \mathbf{u}^h) \, d\mathbf{x} = \ell_{\max}^{n,h}(\delta \mathbf{u}^h, \mathbf{0}, \mathbf{0}), \quad \delta \mathbf{u}^h \in \mathbf{V}_0^h$$

and substituting (20) gives (21a). In the same manner, we obtain (21b) by minimizing

$$J_{\mathbf{g}}^{h,n}(\delta \mathbf{g}_p^h) = J_{\max}^{h,n}(\Delta \mathbf{u}^{h,n}, \Delta \boldsymbol{\varepsilon}_p^{h,n}, \delta \mathbf{g}_p^h), \quad \delta \mathbf{g}_p^h \in \mathbf{G}^h$$

at given $(\Delta \mathbf{u}^{h,n}, \Delta \boldsymbol{\varepsilon}_p^{h,n})$. □

In the fully discrete scheme, all integrals are replaced by a quadrature formula

$$\int_{\Omega} \mathbf{v} \cdot \mathbf{w} \, d\mathbf{x} = \sum_{\boldsymbol{\xi} \in \Xi_h} \omega_{\boldsymbol{\xi}} \mathbf{v}(\boldsymbol{\xi}) \cdot \mathbf{w}(\boldsymbol{\xi}), \quad \mathbf{v}, \mathbf{w} \in \mathbf{V}_h$$

where $\Xi_h \subset \Omega$ are the integration points and $\omega_{\boldsymbol{\xi}}$ the corresponding quadrature weights. Then, the space $\mathbf{E}_h$ is identified with its values at the integration points, i.e. $\mathbf{E}_h = \{\boldsymbol{\varepsilon}_p : \Xi_h \rightarrow \text{sl}(3) \cap \text{Sym}(3)\}$. In the same manner, the discrete return parameter $\gamma^{h,n}$ is approximated in $\Gamma_h = \{\gamma^h : \Xi_h \rightarrow \mathbf{R}\}$ at integration points only. This allows for a point-wise evaluation of the flow rule. We obtain (analogous to Lemma 3) independently for every integration point:

Lemma 9

The discrete dissipation inequality

$$K_0 |\delta \boldsymbol{\varepsilon}_p^h| \geq K_0 |\Delta \boldsymbol{\varepsilon}_p^{h,n}| + \boldsymbol{\alpha}^{h,n} : (\delta \boldsymbol{\varepsilon}_p^h - \Delta \boldsymbol{\varepsilon}_p^{h,n}), \quad \delta \boldsymbol{\varepsilon}_p^h \in \text{sl}(3) \cap \text{Sym}(3) \quad (22)$$

is equivalent to the flow rule

$$\Delta \boldsymbol{\varepsilon}_p^{h,n} = \gamma^{h,n} \frac{\text{dev}(\boldsymbol{\alpha}^{h,n})}{|\text{dev}(\boldsymbol{\alpha}^{h,n})|}, \quad \gamma^{h,n} = |\Delta \boldsymbol{\varepsilon}_p^{h,n}| \quad (23)$$

and the complementary conditions

$$\gamma^{h,n} (|\text{dev}(\boldsymbol{\alpha}^{h,n})| - K_0) = 0, \quad \gamma^{h,n} \geq 0, \quad |\text{dev}(\boldsymbol{\alpha}^{h,n})| \leq K_0 \quad (24)$$

Together, the discrete solution can be obtained by the solution of the finite element problem (21a), (21b) and—independently for every integration point $\boldsymbol{\xi} \in \Xi_h$ —by the flow rule (23) and the complementary conditions (24).

4. ALGORITHMIC NONLOCAL PLASTICITY

In the mixed form we can apply a projection method, where the flow rule and complementary conditions are evaluated by the standard closest point projection [33, Chapter 3.3.2] depending on the actual trial stress, and the result is substituted into the variational problem (21a), (21b). This yields a non-linear system for $(\mathbf{u}^{h,n}, \mathbf{g}_p^{h,n})$, which is solved with a generalized Newton method by substituting the consistent tangent modulus in both equations, linearizing the stress response in (21a) and the strain response in (21b). Note that this results in a fully coupled non-linear

formulation, since a derivative of the projection with respect to both $\boldsymbol{\varepsilon}(\mathbf{u}^h)$ and $\mathbf{g}_p^h$ has to be provided (which makes the realization of such a method quite involved).

Thus, we decided for a modified algorithmic approach. We extend the linearized projection method introduced in [38] to our mixed formulation of nonlocal plasticity: for a given iterate, the flow rule is linearized, so that in every step a linear variational system with linear constraints at the integration points is solved. This subproblem is—due to the constraints—non-linear itself, but the corresponding projections on linear half spaces are easy to compute (in comparison with the fully non-linear constraints).

In order to simplify the notation, we skip in what follows the mesh parameter h .

4.1. The linearized projection method

For fixed values $(\mathbf{u}^{n-1}, \boldsymbol{\varepsilon}_p^{n-1}, \mathbf{g}_p^{n-1}) \in \mathbf{X}(\mathbf{u}_D^{n-1})$ of the preceding time step we consider the incremental problem for the computation of the approximation in step n at time t_n . The linearized projection method iterates on the extended space $\mathbf{Y}^n = \mathbf{X}(\mathbf{u}_D^n) \times \Gamma$, where the linearized parameter is an independent variable.

Substituting the flow function $\phi(\boldsymbol{\alpha}) = |\text{dev}(\boldsymbol{\alpha})| - K_0$ the incremental problem defined by (21a), (21b), (23), (24) is reformulated as follows: find $(\mathbf{u}^n, \boldsymbol{\varepsilon}_p^n, \mathbf{g}_p^n, \gamma^n) \in \mathbf{Y}^n$ with

$$\int_{\Omega} (\boldsymbol{\varepsilon}(\mathbf{u}^n) - \boldsymbol{\varepsilon}_p^n) : \mathbb{C} : \boldsymbol{\varepsilon}(\delta \mathbf{u}) \, d\mathbf{x} = \ell_n(\delta \mathbf{u}), \quad \delta \mathbf{u} \in \mathbf{V}_0 \quad (25a)$$

$$\int_{\Omega} \mathbf{g}_p^n : \mathbb{E}^{-1} : \delta \mathbf{g}_p \, d\mathbf{x} = \int_{\Omega} \boldsymbol{\varepsilon}_p^n : \text{curl}(\delta \mathbf{g}_p) \, d\mathbf{x}, \quad \delta \mathbf{g}_p \in \mathbf{G} \quad (25b)$$

$$\boldsymbol{\varepsilon}_p^n - \boldsymbol{\varepsilon}_p^{n-1} = \gamma^n D\phi(\boldsymbol{\alpha}^n), \quad \boldsymbol{\alpha}^n = \mathbb{C} : (\boldsymbol{\varepsilon}(\mathbf{u}^n) - \boldsymbol{\varepsilon}_p^n) - \mathbb{D} : \boldsymbol{\varepsilon}_p^n - \text{sym}(\text{curl}(\mathbf{g}_p^n)) \quad (25c)$$

$$\gamma^n \phi(\boldsymbol{\alpha}^n) = 0, \quad \gamma^n \geq 0, \quad \phi(\boldsymbol{\alpha}^n) \leq 0 \quad (25d)$$

This non-linear problem (25) is solved iteratively: for an iterate $(\mathbf{u}^{n,k-1}, \boldsymbol{\varepsilon}_p^{n,k-1}, \mathbf{g}_p^{n,k-1}, \gamma^{n,k-1}) \in \mathbf{Y}^n$ of the previous step we define the corresponding relative elastic stress

$$\boldsymbol{\alpha}^{n,k-1} = \mathbb{C} : (\boldsymbol{\varepsilon}(\mathbf{u}^{n,k-1}) - \boldsymbol{\varepsilon}_p^{n,k-1}) - \mathbb{D} : \boldsymbol{\varepsilon}_p^{n,k-1} - \text{sym}(\text{curl}(\mathbf{g}_p^{n,k-1}))$$

and the linearized flow rule

$$\phi_{n,k}(\boldsymbol{\alpha}) = \phi(\boldsymbol{\alpha}^{n,k-1}) + D\phi(\boldsymbol{\alpha}^{n,k-1})(\boldsymbol{\alpha} - \boldsymbol{\alpha}^{n,k-1}) \quad (26)$$

The next iterate $(\mathbf{u}^{n,k}, \boldsymbol{\varepsilon}_p^{n,k}, \mathbf{g}_p^{n,k}, \gamma^{n,k}) \in \mathbf{Y}^n$ is determined as the solution of the linearized system

$$\int_{\Omega} (\boldsymbol{\varepsilon}(\mathbf{u}^{n,k}) - \boldsymbol{\varepsilon}_p^{n,k}) : \mathbb{C} : \boldsymbol{\varepsilon}(\delta \mathbf{u}) \, d\mathbf{x} = \ell_n(\delta \mathbf{u}), \quad \delta \mathbf{u} \in \mathbf{V}_0 \quad (27a)$$

$$\int_{\Omega} \mathbf{g}_p^{n,k} : \mathbb{E}^{-1} : \delta \mathbf{g}_p \, d\mathbf{x} = \int_{\Omega} \boldsymbol{\varepsilon}_p^{n,k} : \text{curl}(\delta \mathbf{g}_p) \, d\mathbf{x}, \quad \delta \mathbf{g}_p \in \mathbf{G} \quad (27b)$$

$$\boldsymbol{\varepsilon}_p^{n,k} - \boldsymbol{\varepsilon}_p^{n-1} = \gamma^{n,k} D\phi(\boldsymbol{\alpha}^{n,k-1}) + \gamma^{n,k-1} D^2\phi(\boldsymbol{\alpha}^{n,k-1}) : (\boldsymbol{\alpha}^{n,k} - \boldsymbol{\alpha}^{n,k-1}) \quad (27c)$$

$$\gamma^{n,k} \phi_{n,k}(\boldsymbol{\alpha}^{n,k}) = 0, \quad \gamma^{n,k} \geq 0, \quad \phi_{n,k}(\boldsymbol{\alpha}^{n,k}) \leq 0 \quad (27d)$$

with $\boldsymbol{\alpha}^{n,k} = \mathbb{C} : (\boldsymbol{\varepsilon}(\mathbf{u}^{n,k}) - \boldsymbol{\varepsilon}_p^{n,k}) - \mathbb{D} : \boldsymbol{\varepsilon}_p^{n,k} - \text{sym}(\text{curl}(\mathbf{g}_p^{n,k}))$, where the derivatives of the flow rule are

$$D\phi(\boldsymbol{\alpha}) = \frac{\text{dev}(\boldsymbol{\alpha})}{|\text{dev}(\boldsymbol{\alpha})|}, \quad D^2\phi(\boldsymbol{\alpha}) : \boldsymbol{\eta} = \frac{\text{dev}(\boldsymbol{\eta})}{|\text{dev}(\boldsymbol{\alpha})|} - \frac{\text{dev}(\boldsymbol{\alpha}) : \text{dev}(\boldsymbol{\eta})}{|\text{dev}(\boldsymbol{\alpha})|^2} \frac{\text{dev}(\boldsymbol{\alpha})}{|\text{dev}(\boldsymbol{\alpha})|}, \quad \boldsymbol{\alpha} \neq \mathbf{0}$$

For the solution of the system (27) we introduce the elastic trial stress

$$\boldsymbol{\theta}_n(\mathbf{u}, \mathbf{g}_p) = \mathbb{C} : (\boldsymbol{\varepsilon}(\mathbf{u}) - \boldsymbol{\varepsilon}_p^{n-1}) - \mathbb{D} : \boldsymbol{\varepsilon}_p^{n-1} - \text{sym}(\text{curl}(\mathbf{g}_p))$$

Lemma 10

Equations (27c) and (27d) have a unique solution

$$\gamma^{n,k} = G_{n,k}(\boldsymbol{\theta}^{n,k}) \quad (28a)$$

$$\boldsymbol{\varepsilon}_p^{n,k} = R_{n,k}(\boldsymbol{\theta}^{n,k}) \quad (28b)$$

depending only on the trial stress $\boldsymbol{\theta}^{n,k} = \boldsymbol{\theta}_n(\mathbf{u}^{n,k}, \mathbf{g}_p^{n,k})$, where the return parameter and the plastic strain response are defined by

$$G_{n,k}(\boldsymbol{\theta}) = \frac{\max\{0, \phi_{n,k}(\boldsymbol{\theta})\}}{(2 + H_0)\mu}$$

$$R_{n,k}(\boldsymbol{\theta}) = \boldsymbol{\varepsilon}_p^{n-1} + \frac{1}{(2 + H_0)\mu} \frac{\gamma^{n,k-1} |\text{dev}(\boldsymbol{\alpha}^{n,k-1})|}{\gamma^{n,k-1} + |\text{dev}(\boldsymbol{\alpha}^{n,k-1})|} D^2\phi(\boldsymbol{\alpha}^{n,k-1}) : \boldsymbol{\theta} + G_{n,k}(\boldsymbol{\theta}) D\phi(\boldsymbol{\alpha}^{n,k-1})$$

Proof

We have $(\mathbb{C} + \mathbb{D}) : (\boldsymbol{\varepsilon}_p^{n,k} - \boldsymbol{\varepsilon}_p^{n-1}) = \boldsymbol{\theta}^{n,k} - \boldsymbol{\alpha}^{n,k}$, and (27c) can be rewritten in the form

$$(\mathbb{C} + \mathbb{D})^{-1} : (\boldsymbol{\theta}^{n,k} - \boldsymbol{\alpha}^{n,k}) = \gamma^{n,k} D\phi(\boldsymbol{\alpha}^{n,k-1}) + \gamma^{n,k-1} D^2\phi(\boldsymbol{\alpha}^{n,k-1}) : (\boldsymbol{\alpha}^{n,k} - \boldsymbol{\alpha}^{n,k-1})$$

This gives (using $D^2\phi(\boldsymbol{\alpha}^{n,k-1}) : \boldsymbol{\alpha}^{n,k-1} = \mathbf{0}$)

$$(\text{id} - (2 + H_0)\mu) \gamma^{n,k-1} D^2\phi(\boldsymbol{\alpha}^{n,k-1}) : \boldsymbol{\alpha}^{n,k} = \boldsymbol{\theta}^{n,k} - (2 + H_0)\mu \gamma^{n,k} D\phi(\boldsymbol{\alpha}^{n,k-1})$$

Substituting (27d) yields $(2 + H_0)\mu \gamma^{n,k} = \max\{0, \phi_{n,k}(\boldsymbol{\theta}^{n,k})\}$ and

$$\boldsymbol{\theta}^{n,k} - \boldsymbol{\alpha}^{n,k} = \frac{\gamma^{n,k-1} |\text{dev}(\boldsymbol{\alpha}^{n,k-1})|}{\gamma^{n,k-1} + |\text{dev}(\boldsymbol{\alpha}^{n,k-1})|} D^2\phi(\boldsymbol{\alpha}^{n,k-1}) : \boldsymbol{\theta}^{n,k} + (2 + H_0)\mu \gamma^{n,k} D\phi(\boldsymbol{\alpha}^{n,k-1})$$

(this can be verified by direct computation; see [38] for details). $\square$

Substituting (28b) into (27a), (27b) results in a variational non-linear problem: find $(\mathbf{u}^{n,k}, \mathbf{g}_p^{n,k})$ such that

$$F_{n,k}(\mathbf{u}^{n,k}, \mathbf{g}_p^{n,k})[\delta\mathbf{u}, \delta\mathbf{g}_p] = \ell_n(\delta\mathbf{u}), \quad (\delta\mathbf{u}, \delta\mathbf{g}_p) \in \mathbf{V}_0 \times \mathbf{G}$$

with

$$F_{n,k}(\mathbf{u}, \mathbf{g}_p)[\delta\mathbf{u}, \delta\mathbf{g}_p] = \int_{\Omega} (\boldsymbol{\varepsilon}(\mathbf{u}) - R_{n,k}(\boldsymbol{\theta}_n(\mathbf{u}, \mathbf{g}_p))) : \mathbb{C} : \boldsymbol{\varepsilon}(\delta\mathbf{u}) \, dx$$

$$+ \int_{\Omega} R_{n,k}(\boldsymbol{\theta}_n(\mathbf{u}, \mathbf{g}_p)) : \text{curl}(\delta\mathbf{g}_p) \, dx - \int_{\Omega} \mathbf{g}_p : \mathbb{E}^{-1} : \delta\mathbf{g}_p \, dx$$

4.2. The consistent tangent operator

The plastic strain response $R_{n,k}(\cdot)$ is only non-linear with respect to the term $\max\{0, \phi_{n,k}(\boldsymbol{\theta})\}$ and therefore a Lipschitz function. Thus, a generalized multi-valued derivative exists (see [39] for the definition and for properties of generalized derivatives). A consistent linearization of the plastic strain response is obtained by the specific choice

$$\begin{aligned} \mathbb{R}_{n,k}(\boldsymbol{\theta}) = & \frac{1}{(2+H_0)\mu} \left(\frac{\gamma^{n,k-1} |\text{dev}(\boldsymbol{\alpha}^{n,k-1})|}{\gamma^{n,k-1} + |\text{dev}(\boldsymbol{\alpha}^{n,k-1})|} D^2 \phi(\boldsymbol{\alpha}^{n,k-1}) \right. \\ & \left. + \text{sgn}(G_{n,k}(\boldsymbol{\theta})) D\phi(\boldsymbol{\alpha}^{n,k-1}) \otimes D\phi(\boldsymbol{\alpha}^{n,k-1}) \right) \in \partial R_{n,k}(\boldsymbol{\theta}) \end{aligned}$$

(see [38] for details on the subdifferential calculus for the computation of consistent tangent operators). Thus, a consistent linearization of $F_{n,k}$ is given by the symmetric bilinear form

$$\begin{aligned} a_{n,k}(\mathbf{u}, \mathbf{g}_p)[(\Delta \mathbf{u}, \Delta \mathbf{g}_p), (\delta \mathbf{u}, \delta \mathbf{g}_p)] \\ = \int_{\Omega} \boldsymbol{\varepsilon}(\Delta \mathbf{u}) : (\mathbb{C} - 4\mu^2 \mathbb{R}_{n,k}(\boldsymbol{\theta})) : \boldsymbol{\varepsilon}(\delta \mathbf{u}) \, d\mathbf{x} + \int_{\Omega} 2\mu \text{curl}(\Delta \mathbf{g}_p) : \mathbb{R}_{n,k}(\boldsymbol{\theta}) : \boldsymbol{\varepsilon}(\delta \mathbf{u}) \, d\mathbf{x} \\ + \int_{\Omega} 2\mu \boldsymbol{\varepsilon}(\Delta \mathbf{u}) : \mathbb{R}_{n,k}(\boldsymbol{\theta}) : \text{curl}(\delta \mathbf{g}_p) \, d\mathbf{x} \\ - \int_{\Omega} (\Delta \mathbf{g}_p : \mathbb{E}^{-1} : \delta \mathbf{g}_p + \text{curl}(\Delta \mathbf{g}_p) : \mathbb{R}_{n,k}(\boldsymbol{\theta}) : \text{curl}(\delta \mathbf{g}_p)) \, d\mathbf{x} \end{aligned}$$

with $\boldsymbol{\theta} = \boldsymbol{\theta}_n(\mathbf{u}, \mathbf{g}_p)$. This results in the following algorithm:

- (S0) Start for $t_0=0$ with $\mathbf{u}^0 = \mathbf{0}$ and $\boldsymbol{\varepsilon}_p^0 = \mathbf{0}$. Set $n = 1$.
- (S1) Choose $(\mathbf{u}^{n,0}, \boldsymbol{\varepsilon}_p^{n,0}, \mathbf{g}_p^{n,0}, \gamma^{n,0}) \in \mathbf{Y}^n$. Set $k = 1$.
- (S2) Set $(\mathbf{u}^{n,k,0}, \mathbf{g}_p^{n,k,0}) = (\mathbf{u}^{n,0}, \mathbf{g}_p^{n,0})$. Set $m = 1$.
- (S3) Evaluate the residual $r_{n,k,m} = \ell_n(\mathbf{u}^{n,k,m-1}) - F_{n,k}(\mathbf{u}^{n,k,m-1}, \mathbf{g}_p^{n,k,m-1})$.
If $\|r_{n,k,m}\|$ is small enough, go to (S5).
- (S4) Assemble the linearization $a_{n,k,m} = a_{n,k}(\mathbf{u}^{n,k,m-1}, \mathbf{g}_p^{n,k,m-1})$.
Compute the Newton update $(\Delta \mathbf{u}^{n,k,m}, \Delta \mathbf{g}_p^{n,k,m})$ by solving

$$a_{n,k,m}[(\Delta \mathbf{u}^{n,k,m}, \Delta \mathbf{g}_p^{n,k,m}), (\delta \mathbf{u}, \delta \mathbf{g}_p)] = r_{n,k,m}[\delta \mathbf{u}, \delta \mathbf{g}_p], \quad (\delta \mathbf{u}, \delta \mathbf{g}_p) \in \mathbf{V}_0 \times \mathbf{G}$$

choose a suitable damping parameter $\rho_{n,k,m} \in (0, 1]$ and set

$$(\mathbf{u}^{n,k,m}, \mathbf{g}_p^{n,k,m}) = (\mathbf{u}^{n,k,m-1}, \mathbf{g}_p^{n,k,m-1}) + \rho_{n,k,m}(\Delta \mathbf{u}^{n,k,m}, \Delta \mathbf{g}_p^{n,k,m})$$

Set $m := m + 1$ and go to (S3).

- (S5) Set $\mathbf{u}^{n,k} = \mathbf{u}^{n,k,m}$, $\mathbf{g}_p^{n,k} = \mathbf{g}_p^{n,k,m}$, $\boldsymbol{\varepsilon}_p^{n,k} = R_{n,k}(\mathbf{u}^{n,k}, \mathbf{g}_p^{n,k})$, $\gamma^{n,k} = G_{n,k}(\mathbf{u}^{n,k}, \mathbf{g}_p^{n,k})$.
Compute $\boldsymbol{\alpha}^{n,k} = \mathbb{C} : (\boldsymbol{\varepsilon}(\mathbf{u}^{n,k}) - \boldsymbol{\varepsilon}_p^{n,k}) - \mathbb{D} : \boldsymbol{\varepsilon}_p^{n,k} - \text{sym}(\text{curl}(\mathbf{g}_p^{n,k}))$.
- (S6) If $\|\boldsymbol{\varepsilon}_p^{n,k} - \boldsymbol{\varepsilon}_p^{n-1} - \gamma^{n,k} D\phi(\boldsymbol{\alpha}^{n,k})\|$ and $\max\{0, \phi(\boldsymbol{\alpha}^{n,k})\}$ are small enough,
set $\mathbf{u}^n = \mathbf{u}^{n,k}$, $\boldsymbol{\varepsilon}_p^n = \boldsymbol{\varepsilon}_p^{n,k}$, $n := n + 1$ and go to (S1).
- (S7) $k := k + 1$ and go to (S2).

In our application, the damping is realized by a simple line search: choose $\rho_{n,k,m} \in \{1, \frac{1}{2}, \frac{1}{4}, \dots\}$ maximal such that $\|r_{n,k,m}\| < \|r_{n,k,m-1}\|$. For sufficiently small Δt_n , we have $\rho_{n,k,m} = 1$ in most cases.

5. NUMERICAL EXPERIMENTS

In this section we discuss numerical test calculations for the evaluation of the regularizing properties of the nonlocal model. The computations are realized in the parallel finite element code M++ [40]. Note that all our discretizations and all non-linear and linear solution methods are provided in a general manner and do not specifically depend on the studied representative model; they easily transfer to other nonlocal models without substantial changes.

5.1. An example configuration

For the numerical test we consider a traction problem where the load functional

$$\ell(t, \delta \mathbf{u}) = t \int_{\Gamma_N} \mathbf{t}_N \cdot \delta \mathbf{u} \, da, \quad \mathbf{t}_N = (0, 0, 1)^T$$

depends linearly on the loading parameter t (see Figure 1 for some configuration details).

5.2. Reparametrization

Since this model is rate independent, the parameter t has no direct link to the physical time. Here we are interested in the regularization properties of the local hardening parameters H_0 and the nonlocal plastic length scale L_c , so that we will evaluate the model close to the limit load of the

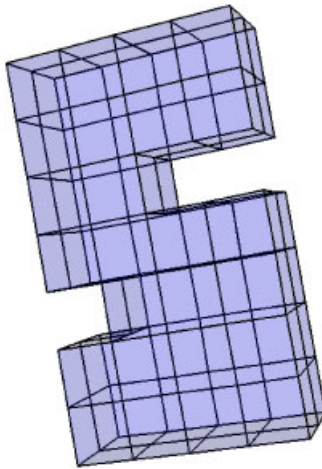


Figure 1. Initial configuration $\Omega \subset (0, 4) \times (0, 1) \times (0, 7)$. On the bottom $\Gamma_D = (0, 4) \times (0, 1) \times \{0\}$ the body is fixed (homogeneous Dirichlet boundary conditions $\mathbf{u}_D \equiv \mathbf{0}$ on Γ_D), a traction force is applied on the top surface $\Gamma_N = (0, 4) \times (0, 1) \times \{7\}$. Material parameters: the Poisson ratio $\nu = 0.29$, Young's modulus $E = 206900.00$ (N/mm²), yield stress $K_0 = 450.00$ (N/mm²).

model of perfect plasticity. For small hardening the model is quite sensitive, when the loading parameter t is close to the limit load. This can be easily avoided by the following reparametrization.

We consider a load cycle with $2N$ loading steps using uniform steps $s_n = n\Delta s$, $n = 1, \dots, N$ with a fixed increment $\Delta s = S/N$ and $s_n = S - (n - N)\Delta s$, $n = N + 1, \dots, 2N$. In our tests we use $S = 0.6$ and $N = 60$. For every parameter s_n we compute t_n such that the external work satisfies

$$\ell(t_n, \mathbf{u}^n) = s_n \quad (29)$$

Therefore, in every step of the non-linear iteration we now solve the following problem: find $(\mathbf{u}^{n,k}, \mathbf{g}_p^{n,k}, t_{k,n})$ such that

$$F_{n,k}(\mathbf{u}^{n,k}, \mathbf{g}_p^{n,k})[\delta \mathbf{u}, \delta \mathbf{g}_p] = \ell(t_{n,k}, \delta \mathbf{u}), \quad (\delta \mathbf{u}, \delta \mathbf{g}_p) \in \mathbf{V}_0 \times \mathbf{G}$$

subject to the linear constraint $\ell(t_{n,k}, \mathbf{u}^{n,k}) = s_n$.

Thus, for the iterate $(\mathbf{u}^{n,k,m-1}, \mathbf{g}_p^{n,k,m-1}, t_{k,n,m-1})$ in (S3) we compute the modified residual

$$r_{n,k,m} = \ell(t_{n,k,m-1}, \delta \mathbf{u}) - F_{n,k}(\mathbf{u}^{n,k,m-1}, \mathbf{g}_p^{n,k,m-1})$$

and in (S4) the following saddle point problem is solved: find $(\Delta \mathbf{u}^{n,k,m}, \Delta \mathbf{g}_p^{n,k,m}, \Delta t_{k,n,m})$ such that

$$a_{n,k,m}[(\Delta \mathbf{u}^{n,k,m}, \Delta \mathbf{g}_p^{n,k,m}), (\delta \mathbf{u}, \delta \mathbf{g}_p)] + \ell(\Delta t_{k,n,m}, \delta \mathbf{u}) = r_{n,k,m}[\delta \mathbf{u}, \delta \mathbf{g}_p] \quad (30a)$$

$$\ell(\delta t, \Delta \mathbf{u}^{n,k,m}) = s_n - \ell(t_{n,k,m-1}, \mathbf{u}^{n,k,m-1}) \quad (30b)$$

for all $(\delta \mathbf{u}, \delta \mathbf{g}_p) \in \mathbf{V}_0 \times \mathbf{G}$ and $\delta t \in \mathbf{R}$.

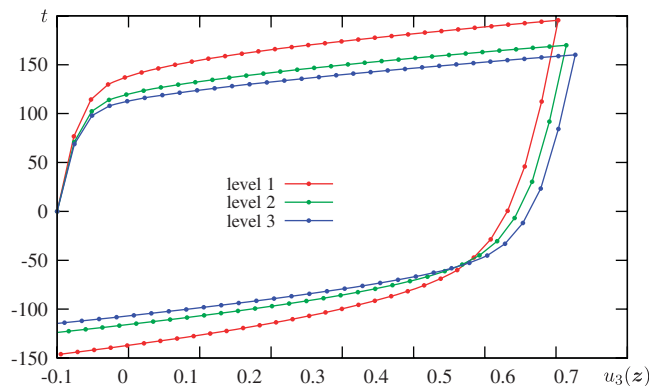


Figure 2. Convergence study of the load–displacement curve for levels 1–3 with 400, 3200, 25 600 cells (6904, 46 420 and 338 500 degrees of freedom) for $L_c = 0.01$ and $H_0 = 0.001$. Here, the load is proportional to t , and the displacement $\mathbf{u} = (u_1, u_2, u_3)$ is given at the point $\mathbf{z} = (0, 0, 7)^T$.

5.3. Solution of the linearized system

The linear system (30) has the form

$$\begin{pmatrix} K & \ell \\ \ell^T & 0 \end{pmatrix} \begin{pmatrix} x \\ t \end{pmatrix} = \begin{pmatrix} r \\ q \end{pmatrix}$$

with $K \in \mathbf{R}^{N_h \times N_h}$, $\ell \in \mathbf{R}^{N_h}$, where $N_h = \dim \mathbf{X}^h$. This bordered linear system is resolved by the following algorithm:

$$\text{solve } Kc = \ell \tag{31a}$$

$$\text{set } t = (c^T r - q) / (c^T \ell) \tag{31b}$$

$$\text{solve } Kx = r - t\ell \tag{31c}$$

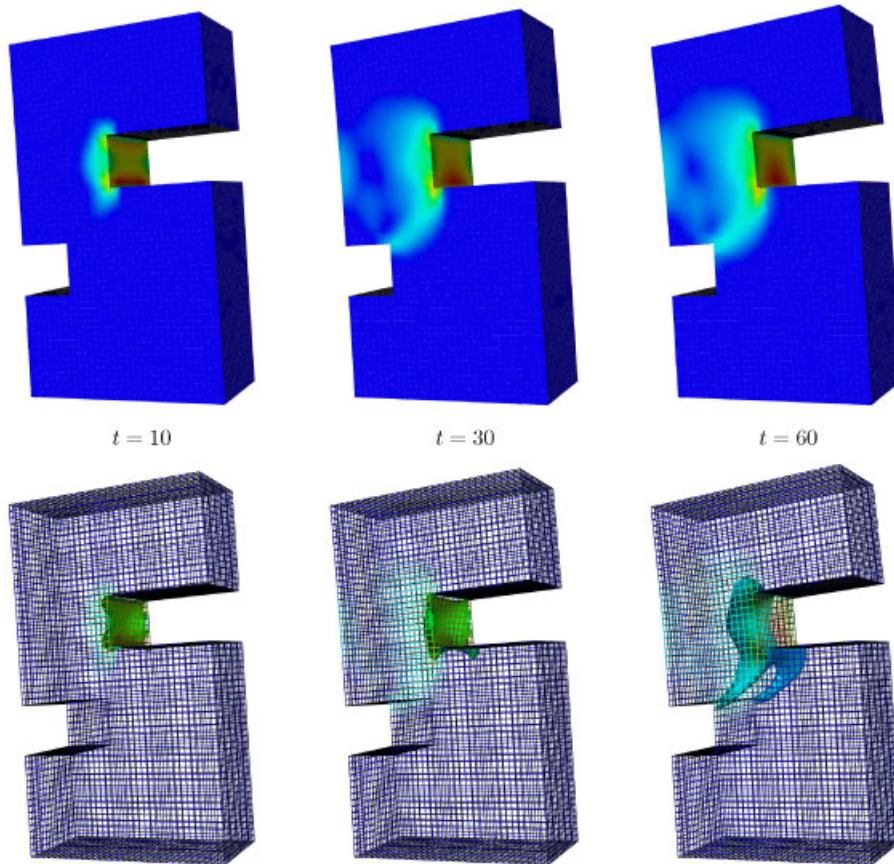


Figure 3. Distribution of the plastic strain on the boundary and on an isosurface for the nonlocal model ($L_c=0.01$ and $H_0=0.001$).

For the solution of the two linear subproblems (31a) and (31b) we use a parallel Krylov method [41] accelerated with a multilevel ILU preconditioner with pivoting and dropping strategy by Mayer [42, 43]. Note that the matrix $K = \begin{pmatrix} A & B \\ B^T & -C \end{pmatrix}$ is symmetric, invertible but indefinite (A and C are symmetric positive definite), so that simple cg-iterations with standard preconditioners do not apply.

5.4. Convergence properties

The result for a sample computation is illustrated in Figure 3, and in Figure 2 we present the convergence with respect to the mesh size for fixed parameters $H_0 > 0$ and $L_0 > 0$.

In this experiment we observe linear convergence with respect to h , which is realistic for lowest order elements. Because of the reparametrization and the sufficiently small choice of the increment parameter Δs , we always observe local quadratic convergence of the non-linear scheme; a typical convergence history is illustrated in Table I.

5.5. Evaluation of the parameter dependence

Finally, we consider the dependence of the results on the nondimensional hardening parameter H_0 and the plastic length scale L_c in Figure 4. Here, we observe clearly that both kinematic hardening and gradient plasticity have a regularizing effect and can be used (for small parameters) to substitute the not well-posed model of perfect plasticity. In particular, we observe that the nonlocal plasticity already has strong regularization effect even with very small kinematic hardening. Moreover, we observe stable convergence and approximation properties for all tested parameters, so that the

Table I. Non-linear convergence of the linearized projection method in loading step $n=32$ on level 2 with 3200 cells.

k	m	$\ r_{n,k,m}\ $	$\max\{\phi(\sigma^{n,k,m}), 0\}$	$\ \epsilon_p^{n,k} - \epsilon_p^{n-1} - \gamma^{n,k} D\phi(\alpha^{n,k})\ $
0	0	0.00000000	0.94854414	0.0000042244
1	1	11.53189802		
1	2	0.11205330		
1	3	0.00324081		
1	4	0.00000032	0.12747705	0.0000035837
2	1	0.01711659		
2	2	0.00003864		
2	3	ε	0.00001832	ε
3	1	0.00000292		
3	2	ε	ε	ε

The iteration is started with the extrapolated solution from the previous loading step. Thus, the initial residual vanishes in the equilibrium equation. Here, we need three steps in the linearized projection method, where projection onto the linear half space requires 4, 3 and 2 generalized Newton steps. The iteration is stopped for $\varepsilon < 10^{-9}$. Note that the algebraic error in this non-linear test is far smaller than the approximation error of the finite element scheme.

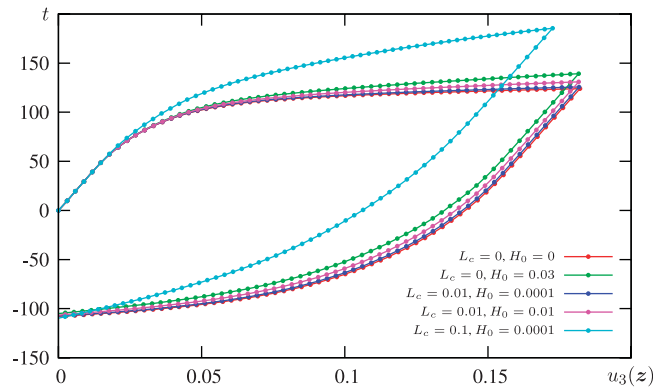


Figure 4. Load–displacement curves for the three different models: perfect plasticity ($L_c=0$ and $H_0=0$), kinematic hardening (local plasticity with $L_c=0$), and the nonlocal model with three different parameters (H_0, L_c). Here, we use 3200 cells on level 2, and again the displacement is given for the point $\mathbf{z}=(0, 0, 7)^T$.

new model is now ready to use in the context of experimental data fitting or for the extension to geometrically non-linear models. Both will be the topics for further research.

Comparing with the results in Figures 2 and 4 we observe, in addition, that for coarse meshes the regularization effect caused by the FEM-discretization dominates over the regularization due to the material model; this indicates that the evaluation of regularization effects indeed requires powerful numerical methods, otherwise it is not possible to separate clearly between discretization effects and material properties.

Remark 11

Our model does not feature plastic spin; this would require to consider nonsymmetric plastic distortions $\mathbf{p}$ as well. The difficulty that one encounters for this extension is tied to the fact that coercivity is not obtained in known Hilbert spaces such as $H(\text{curl})$ since only the symmetric part of the plastic distortion is an $L_2(\Omega)$ -function *a priori*, so that a suitable analytical framework has to be developed.

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