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On the superlinear convergence in computational elasto-plasticity

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Abstract

We consider the convergence properties of return algorithms for a large class of rate-independent plasticity models. Based on recent results for semismooth functions, we can analyze these algorithms in the context of semismooth Newton methods guaranteeing local superlinear convergence. This recovers results for classical models but also extends to general hardening laws, multi-yield plasticity, and to several non-associated models. The superlinear convergence is also numerically shown for a large-scale parallel simulation of Drucker-Prager elasto-plasticity.

Keywords: computational plasticity, return mapping algorithms, semismooth Newton methods, non-associated plasticity

1. Introduction

A key result in computational plasticity is obtained in the seminal paper Simo and Taylor (1985), where simple radial return algorithms are generalized to a large class of plasticity models, and where superlinear convergence is observed using the corresponding algorithmically consistent tangent. This result extends earlier work by, e.g., Wilkins (1964); Krieg and Key (1976), and it is complemented by Simo et al. (1988a) for multi-yield plasticity. Afterwards, the underlying ideas have been applied to a broad range of applications (e.g., Borja and Lee, 1990; Hofstetter et al., 1993); also see the references in Simo and Hughes (1998).

Meanwhile, the application of return mappings is the standard computational approach. They are based on the following strategy: if the trial stress is admissible, the response is elastic. Otherwise, the trial stress has to be “returned” to the admissible set. In the latter case, not only a nonlinear system of equations has to be solved, but also the set of active constraints has to be identified. Whereas the identification process is trivial for single-yield models, the situation is more complex for multi-yield problems. In many applications, the structure of the equations allows for efficient solution methods which are mainly based on Newton’s method (possibly applied on a reduced system). Once the incremental stress response is computed, the algorithmically consistent tangent is defined as the derivative of the stress response with respect to the trial stress (depending on the formulation it may also be the derivative w.r.t. the strain increment). The resulting algorithms perform very well in practice and yield fast nonlinear convergence of the (outer) Newton iteration.

However, as rate-independent plasticity is inherently nonsmooth, the observed convergence properties cannot be explained by the standard Newton theory. Concerning convergence properties of return algorithms, only a few results are available. E.g., in Blaheta (1997) quadratic convergence is shown if the active set of plastic material points is correctly

identified, and Albery, Carstensen, and Zarrabi 1999 show global convergence of a suitably damped generalized Newton methods for simple associated plasticity models.

Only recently, plasticity has been analyzed in the context of semismooth Newton methods (Hager and Wohlmuth, 2009; Gruber and Valdman, 2009). These results consider simple models, where explicit formulae for the closest point projection are at hand, so that semismoothness can be checked directly by a reformulation using nonlinear complementarity functions as it is done in Hager and Wohlmuth (2009).

In this work we aim for the development of a general framework for the construction and semismooth analysis of return algorithms. In particular, we consider rate-independent models (and its viscous Duvault-Lions regularizations) of associated plasticity with general nonlinear hardening, and three different non-associated models (including multi-yield flow functions); for all these cases we are able to prove local superlinear convergence. Our algorithm to determine the stress response also facilitates the computation of the corresponding consistent tangent operator. However, we remark that for very specific applications often simpler ways for the evaluation of the stress response are at hand (e.g., the nonlinear system can be reduced to a scalar equation for the consistency parameter). Nevertheless, our algorithm is simple to implement and applicable to a wide range of applications. In single-yield models, we re-obtain the classical formulas as presented, e.g., in (Simo and Hughes, 1998, Section 3.6).

Our results strongly rely on nonsmooth analysis which itself is heavily influenced by the fields of optimization theory and complementarity problems. This seems reasonable since in rate-independent plasticity, plastic flow is typically characterized by complementarity conditions. Moreover, for associated material models, it is known that the stress response corresponds to the solution of a minimization problem. Building blocks of this nonsmooth calculus are (typically set-valued) generalized derivatives like Clarke’s generalized Jacobian or

the B(ouligand)-subdifferential, cf. Clarke (1983), which can then be used to define corresponding generalized Newton methods for nonsmooth problems. In the context of proving superlinear convergence of such methods, the notion of semismooth functions (Mifflin, 1977; Qi and Sun, 1993) is of particular importance. Nevertheless, it turns out that the classical results on semismooth functions are not sufficient for a general analysis of return algorithms. Only recently, suitable extensions of the implicit function theorem to the semismooth case were obtained in (Gowda, 2004; von Heusinger and Kanzow, 2008), which play a crucial role in our applications. The new result on the semismoothness of the orthogonal projection onto second order unit cones (Hayashi et al., 2005; Goh and Meng, 2006) applies to Drucker-Prager plasticity.

The paper is organized as follows. In Section 2, we start with the equations of quasi-static elasto-plasticity and suitable discretizations in time (by backward differences - leading to the incremental setting) and space (by the finite element method). Introducing the *(incremental) stress response function* allows to reformulate the incremental problem as a second order partial differential equation. Section 3 then sets the focus on generalized Newton methods based on the nonsmooth calculus. The abstract framework is then applied to various examples. First, we consider standard problems in associated plasticity in sections 4 and 5. Then, we focus on non-associated models, mainly motivated by soil mechanics. In Section 6, we analyze Drucker-Prager plasticity as well as a smoothed variant. The latter also shows that the active set method proposed in Section 3 resembles the well-known formulas for the consistent tangent when applied to a single-yield model. In sections 7 and 8, we consider two problems in soil mechanics, the modified Cam-clay model and the (multi-yield) cap-model, for which existence and uniqueness results concerning the underlying initial boundary value problems have only been obtained recently, cf. Dal Maso and DeSimone (2009); Dal Maso et al. (2011); Babadjian et al. (2011). Finally, we present numerical experiments with Drucker-Prager plasticity which verify our theoretical results even for very large problems with several million degrees of freedom.

2. Problem setting

Let $\Omega \subset \mathbb{R}^d$, $d \in \{2, 3\}$ be the body of interest, let $\Gamma_D \subset \partial\Omega$ be the Dirichlet part of the boundary where we prescribe a displacement \mathbf{u}_D , and let $\Gamma_N = \partial\Omega \setminus \Gamma_D$ be the Neumann part where a traction force is applied. The Cauchy stress tensor $\boldsymbol{\sigma}(x, t)$ is required to be in equilibrium with the external forces, i.e. for a given body force (density) $\mathbf{b}: \Omega \times [0, T] \rightarrow \mathbb{R}^d$ and a traction force (density) $\mathbf{t}_N: \Gamma_N \times [0, T] \rightarrow \mathbb{R}^d$, we require

$$\begin{aligned} -\operatorname{div} \boldsymbol{\sigma}(x, t) &= \mathbf{b}(x, t) \quad \text{in } \Omega, \\ \boldsymbol{\sigma}(x, t)\mathbf{n}(x) &= \mathbf{t}_N(x, t) \quad \text{on } \Gamma_N. \end{aligned} \quad (2.1)$$

Balance of angular momentum implies symmetry of $\boldsymbol{\sigma}$, i.e.

$$\boldsymbol{\sigma}(x, t) \in S := \{\boldsymbol{\eta} \in \mathbb{R}^{d,d} : \boldsymbol{\eta} = \boldsymbol{\eta}^T\},$$

where S denotes the symmetric second order tensors. In the following, we will mostly omit the dependence on (x, t) whenever we consider relations which hold point-wise in space and/or at a fixed time instance.

In this work we only consider the small strain setting, i.e., the stress-strain relation is given by Hooke's law

$$\boldsymbol{\sigma} = \mathbb{C}[\boldsymbol{\varepsilon}(\mathbf{u}) - \boldsymbol{\varepsilon}_p] \quad (2.2)$$

with the fourth order linear elasticity tensor $\mathbb{C} \in \operatorname{Lin}(S, S)$ which is assumed to be symmetric and positive definite. For a given displacement \mathbf{u} , $\boldsymbol{\varepsilon}(\mathbf{u}) = \frac{1}{2}(\mathbf{D}\mathbf{u} + \mathbf{D}\mathbf{u}^T) \in S$ is the total strain, and $\boldsymbol{\varepsilon}_p \in S$ is the plastic strain. For isotropic materials, Hooke's law has the form $\boldsymbol{\sigma} = \mathbb{C}[\boldsymbol{\varepsilon}] = 2\mu \operatorname{dev}(\boldsymbol{\varepsilon}) + \kappa \operatorname{tr}(\boldsymbol{\varepsilon})\mathbf{1}$, with the shear modulus $\mu > 0$ and the bulk modulus $\kappa > 0$; $\mathbf{1}$ denotes the second order unit tensor. By $\operatorname{dev}(\cdot)$, we denote the orthogonal projection onto the deviatoric subspace $S_0 = \{\boldsymbol{\sigma} \in S : \operatorname{tr}(\boldsymbol{\sigma}) = 0\} \subset S$ w.r.t. the Frobenius inner product $\boldsymbol{\sigma} : \boldsymbol{\varepsilon} = \sum_{i,k=1}^d \sigma_{ik} \varepsilon_{ik}$.

2.1. Quasi-static elasto-plasticity

The plastic evolution is described by the plastic strain $\boldsymbol{\varepsilon}_p$, and—in most cases—by further internal variables $\boldsymbol{\eta}$. Together with the Cauchy stress they build the generalized stress space

$$\mathcal{S} = S \times \mathbb{R}^m, \quad \Sigma = (\boldsymbol{\sigma}, \boldsymbol{\eta}) \in \mathcal{S}.$$

The number $m \in \mathbb{N}$ of internal variables depends on the context. Please note that $\boldsymbol{\eta}$ is not necessarily a thermodynamic stress, but for the ease of notation, we treat it like a stress.

In *rate-independent* elasto-plasticity, time is merely a path variable than a physical quantity, i.e. the system is invariant under temporal rescaling (a mathematically precise definition is given in Mielke (2005)). The generalized stress Σ is said to be *admissible* if it satisfies

$$\Sigma \in K := \{\hat{\Sigma} \in \mathcal{S} : f_i(\hat{\Sigma}) \leq 0 \text{ for } i = 1, \dots, p\}$$

for given *yield functions* $f_i: \mathcal{S} \rightarrow \mathbb{R}$. The path-/time-dependency is reflected by an evolution law for the plastic strain rate $\dot{\boldsymbol{\varepsilon}}_p$ which is functionally related to the current stress state Σ . In rate-independent plasticity, this relation is typically given in the form

$$\dot{\boldsymbol{\varepsilon}}_p = \sum_{i=1}^p \lambda_i \mathbf{r}_i(\Sigma), \quad (2.3)$$

with prescribed plastic flow directions $\mathbf{r}_i: \mathcal{S} \rightarrow S$ (possibly multi-valued) and the consistency parameters $\lambda_i \geq 0$ (also called plastic or Lagrange multipliers). In multi-yield plasticity ($p > 1$), this form of the flow rule is often attributed to Koiter (1960).

For the internal variables $\boldsymbol{\eta}$ (e.g. related with hardening), a corresponding law has to be established. We consider two different cases. For standard materials, the evolution laws can be written as

$$\dot{\boldsymbol{\eta}} = \sum_{i=1}^p \lambda_i \mathbf{h}_i(\Sigma) \quad (2.4)$$

with given functions $\mathbf{h}_i: \mathcal{S} \rightarrow \mathbb{R}^m$. Note that hardening laws are often formulated in terms of variables $\boldsymbol{\delta} \in \mathbb{R}^m$ which are thermodynamically conjugate to $\boldsymbol{\eta}$. But as we present return algorithms in the stress-space, we will formulate the equation w.r.t. the generalized stress $\Sigma = (\boldsymbol{\sigma}, \boldsymbol{\eta})$.

In a second application class, the internal variables are determined by suitable state equations, e.g., for the modified Cam-clay or the cap-model in sections 7 and 8.

In the rate-independent case, the consistency parameters λ_i are determined by the complementarity conditions in Karush-Kuhn-Tucker (KKT) form, i.e.,

$$0 = \lambda_i f_i(\Sigma), \quad \lambda_i \geq 0, \quad f_i(\Sigma) \leq 0,$$

for $i = 1, \dots, p$.

If the generalized flow directions (\mathbf{r}, \mathbf{h}) are determined as the derivative of the yield function f , we speak of an *associated flow rule*. In this work, the associated flow rule means that both the plastic strain rate and the law for the internal variables are derived from the yield functions f_i . This differs from the convention sometimes used in soil mechanics, where the flow rule is often said to be associated if only $\dot{\boldsymbol{\varepsilon}}_p = \sum \lambda_i D_{\boldsymbol{\sigma}} f_i(\Sigma)$.

We also consider *rate-dependent* visco-plasticity in the sense of Duvault-Lions (Duvaut and Lions, 1976; Simo and Hughes, 1998). Denoting by $\bar{\Sigma} = (\bar{\boldsymbol{\sigma}}, \bar{\boldsymbol{\eta}})$ the solution of rate-independent plasticity, the flow rule takes the form

$$\dot{\boldsymbol{\varepsilon}}_p = \frac{1}{\beta} \mathbb{C}^{-1}[\boldsymbol{\sigma} - \bar{\boldsymbol{\sigma}}], \quad (2.5)$$

depending on some relaxation parameter $\beta > 0$ (and similarly for the internal variables if present).

For single-yield models, return algorithms can also be formulated for visco-plastic models of Perzyna type. Here, we only consider the generalized Duvaut-Lions model, as it is also meaningful in multi-yield plasticity (Simo et al., 1988a).

2.2. Incremental plasticity

We introduce a time discretization of the interval $[0, T]$ by using the partition $0 = t_0 < t_1 < \dots < t_N = T$ and set $\Delta t_n = t_n - t_{n-1}$. Temporal derivatives are approximated by backward differences, e.g. $\dot{\boldsymbol{\varepsilon}}_p(t_n) \approx \frac{1}{\Delta t_n}(\boldsymbol{\varepsilon}_p^n - \boldsymbol{\varepsilon}_p^{n-1})$. This results in the incremental flow rule as

$$\boldsymbol{\varepsilon}_p^n = \boldsymbol{\varepsilon}_p^{n-1} + \sum_{i=1}^p \Delta \lambda_i^n \mathbf{r}_i(\Sigma^n), \quad (2.6)$$

where we set $\Delta \lambda_i^n = \Delta t_n \lambda_i^n$. Substitution into Hooke's law gives

$$\begin{aligned} \boldsymbol{\sigma}^n &= \mathbb{C}[\boldsymbol{\varepsilon}(\mathbf{u}^n) - \boldsymbol{\varepsilon}_p^{n-1}] - \sum_{i=1}^p \Delta \lambda_i^n \mathbb{C}[\mathbf{r}_i(\Sigma^n)] \\ &= \boldsymbol{\sigma}_{\text{tr}} - \sum_{i=1}^p \Delta \lambda_i^n \mathbb{C}[\mathbf{r}_i(\Sigma^n)]. \end{aligned} \quad (2.7)$$

with the *trial stress* $\boldsymbol{\sigma}_{\text{tr}} = \mathbb{C}[\boldsymbol{\varepsilon}(\mathbf{u}^n) - \boldsymbol{\varepsilon}_p^{n-1}]$. Similarly, we obtain the incremental law for the internal variables, e.g., for linear kinematic or isotropic hardening we can find

$$\boldsymbol{\eta}^n = \boldsymbol{\eta}^{n-1} + \sum_{i=1}^p \Delta \lambda_i \mathbf{h}_i(\Sigma^n). \quad (2.8)$$

In other cases, e.g. the modified Cam-clay model, the hardening law has to be modified accordingly.

The consistency parameter is determined by the incremental complementarity conditions

$$0 = \Delta \lambda_i^n f_i(\Sigma^n), \quad \Delta \lambda_i^n \geq 0, \quad f_i(\Sigma^n) \leq 0, \quad (2.9)$$

for $i = 1, \dots, p$. Together, (2.7), (2.9) and the incremental law for the internal variables, e.g. (2.8), implicitly define the return mapping, i.e. they determine Σ^n and $\Delta \lambda_i^n$ in terms of the trial stress $\boldsymbol{\sigma}_{\text{tr}}$ and history parameters $\boldsymbol{\eta}^{n-1}$ at time t_{n-1} .

Our objective is to construct and to analyze the smoothness of incremental generalized stress response functions

$$\mathcal{R}^n = (R^n, E^n) : \mathcal{S} \rightarrow \mathcal{S}, \quad \Sigma^n = \mathcal{R}^n(\boldsymbol{\sigma}_{\text{tr}}), \quad (2.10)$$

so that the first component $\boldsymbol{\sigma}^n = R^n(\boldsymbol{\sigma}_{\text{tr}})$ is the return mapping for the Cauchy stress, and the second component $\boldsymbol{\eta}^n = E^n(\boldsymbol{\sigma}_{\text{tr}})$ determines the update of the history variables.

By means of the stress response function, the incremental elasto-plasticity problem can be reformulated as a nonlinear second order partial differential equation: depending on $\boldsymbol{\varepsilon}_p^{n-1}$ and $\boldsymbol{\eta}^{n-1}$ find $\boldsymbol{\sigma}^n$ and \mathbf{u}^n such that

$$-\text{div } \boldsymbol{\sigma}^n(x) = \mathbf{b}(x, t_n), \quad x \in \Omega, \quad (2.11a)$$

$$\boldsymbol{\sigma}^n(x) = R^n(\mathbb{C}[\boldsymbol{\varepsilon}(\mathbf{u}^n(x)) - \boldsymbol{\varepsilon}_p^{n-1}(x)]), \quad x \in \Omega, \quad (2.11b)$$

$$\mathbf{u}^n(x) = \mathbf{u}_D(x, t_n), \quad x \in \Gamma_D, \quad (2.11c)$$

$$\boldsymbol{\sigma}^n(x) \mathbf{n}(x) = \mathbf{t}_N(x, t_n), \quad x \in \Gamma_N. \quad (2.11d)$$

The incremental solution then defines the plastic strain and the new history variables by

$$\boldsymbol{\varepsilon}_p^n(x) = \boldsymbol{\varepsilon}(\mathbf{u}^n(x)) - \mathbb{C}^{-1}[\boldsymbol{\sigma}^n(x)], \quad x \in \Omega, \quad (2.12a)$$

$$\boldsymbol{\eta}^n(x) = E^n(\mathbb{C}[\boldsymbol{\varepsilon}(\mathbf{u}^n(x)) - \boldsymbol{\varepsilon}_p^{n-1}(x)]), \quad x \in \Omega. \quad (2.12b)$$

Remark 2.1. *It is not a priori clear that the nonlinear system (2.11) is well-posed, and in particular for non-associated models even the existence of a solution (in an appropriate weak sense) cannot be guaranteed in all cases (Dal Maso and DeSimone, 2009; Dal Maso et al., 2011; Babadjian et al., 2011). Below, we will refer to known existence results which strongly depend on the model under consideration. Here, we will study a finite element approximation of this system, and we always assume that a solution exists.*

2.3. Discretization by the Finite Element Method

The finite element discretization is based on the weak formulation of (2.11): find \mathbf{u}^n satisfying the boundary condition (2.11c) and such that

$$\int_{\Omega} R^n(\mathbb{C}[\boldsymbol{\varepsilon}(\mathbf{u}^n) - \boldsymbol{\varepsilon}_p^{n-1}]) : \boldsymbol{\varepsilon}(\mathbf{w}) \, dx - \ell^n(\mathbf{w}) = 0 \quad (2.13)$$

holds for all test functions \mathbf{w} with $\mathbf{w}|_{\Gamma_D} = 0$; the load functional is given by

$$\ell^n(\mathbf{w}) \equiv \ell(t_n, \mathbf{w}) = \int_{\Omega} \mathbf{b}(t_n) \cdot \mathbf{w} \, dx + \int_{\Gamma_N} \mathbf{t}_N(t_n) \cdot \mathbf{w} \, da. \quad (2.14)$$

The solution \mathbf{u}^n of the nonlinear variational problem (2.13) then defines the Cauchy stress by (2.11b) and the history update (2.12).

Let Ω be polygonal with a triangulation $\bar{\Omega} = \cup_{T \in \mathcal{M}} T$; where \mathcal{M} denotes the set of mesh cells. The standard approach in computational elasto-plasticity is to approximate the displacement by Lagrange finite elements

$$\begin{aligned} \mathbf{X}_h(\mathbf{u}_D) &= \{\mathbf{u}_h \in C^{0,1}(\Omega, \mathbb{R}^d) : \mathbf{u}_h|_T \in \mathbb{P}_k, T \in \mathcal{M}, \\ &\quad \mathbf{u}_h(x) = \mathbf{u}_D(x), x \in \mathcal{D}\}, \end{aligned}$$

where $\mathcal{D} \subset \Gamma_D$ are the nodal points on the Dirichlet boundary $\Gamma_D \subset \partial\Omega$; we simply write $\mathbf{X}_h = \mathbf{X}_h(0)$. Now, the incremental finite element problem reads as follows: find $\mathbf{u}_h^n \in \mathbf{X}_h(\mathbf{u}_D)$ such that

$$\int_{\Omega} R^n(\mathbb{C}[\boldsymbol{\varepsilon}(\mathbf{u}_h^n) - \boldsymbol{\varepsilon}_p^{n-1}]) : \boldsymbol{\varepsilon}(\mathbf{w}_h) dx = \ell^n(\mathbf{w}_h), \quad \mathbf{w}_h \in \mathbf{X}_h. \quad (2.15)$$

Our objective is to study the local convergence of generalized Newton methods for the discrete nonlinear equation (2.15).

Remark 2.2. *For associated materials, it is possible to define a (global) minimization problem for which (2.11) are just the optimality conditions. Then, powerful methods from optimization are available, e.g., SQP methods (Wieners, 2007, 2008), interior point methods (Krabbenhoft, Lyamin, Sloan, and Wriggers, 2006), and augmented Lagrange methods (Sauter, 2010). For these methods, global convergence can be guaranteed.*

Remark 2.3. *For lowest order discretization on simplices, strains and stresses are constant in the cells T , and all integrals can be evaluated exactly. In general, all integrals are approximated by quadrature formulas, and then the return algorithm is evaluated in every integration point. For simplicity of the notation, we still use integrals although in praxis they are approximated by quadrature.*

From now on, as we will always consider the incremental setting, we often omit the superscripts $(\cdot)^n$ and time instances and we always consider the time step from t_{n-1} to t_n . History variables at time t_{n-1} will be indicated by a superscript $(\cdot)^{\text{old}}$ in the following.

3. The generalized Newton method

In general, we cannot expect that the response function is differentiable. Thus, an extended concept of differentiability is required in order to construct Newton type methods for the solution of incremental plasticity in the form (2.15). A suitable framework is provided by the introduction of set-valued generalized derivatives and corresponding generalized Newton algorithms. Such methods are elaborately studied in the context of (nonsmooth) optimization (Klatte and Kummer, 2002; Pang and Facchinei, 2003a,b). A short compilation of known results, together with a short list of suitable references, is given in the appendix.

In the following we assume that the response function for the Cauchy stress $R : S \rightarrow S$ is (locally) Lipschitz continuous. This implies that R is differentiable almost everywhere, i.e., the set $\Theta_R := \{\boldsymbol{\theta} \in S : R \text{ is differentiable at } \boldsymbol{\theta}\}$ is dense in S . The set-valued Bouligand-subdifferential of R is given as

$$\partial^B R(\boldsymbol{\sigma}_{\text{tr}}) = \{\mathbb{S} \in \text{Lin}(S, S) : \mathbb{S} = \lim_{\boldsymbol{\theta} \rightarrow \boldsymbol{\sigma}_{\text{tr}}, \boldsymbol{\theta} \in \Theta_R} DR(\boldsymbol{\theta})\},$$

and Clarke's subdifferential is its convex hull

$$\partial R(\boldsymbol{\sigma}_{\text{tr}}) = \text{conv} \{\partial^B R(\boldsymbol{\sigma}_{\text{tr}})\}.$$

Moreover, we assume that R is *semismooth* for all $\boldsymbol{\sigma}_{\text{tr}}$, i.e., we assume that for any $\mathbb{S} \in \partial R(\boldsymbol{\sigma}_{\text{tr}} + \boldsymbol{\theta})$:

$$|\mathbb{S}(\boldsymbol{\sigma}_{\text{tr}} + \boldsymbol{\theta}) - R(\boldsymbol{\sigma}_{\text{tr}}) - \mathbb{S}[\boldsymbol{\theta}]| = o(|\boldsymbol{\theta}|) \quad \text{as } \boldsymbol{\theta} \rightarrow 0 \quad (3.1)$$

is satisfied. If $o(|\boldsymbol{\theta}|)$ can be replaced by $O(|\boldsymbol{\theta}|^{1+s})$, we call R *semismooth of order $s \in (0, 1]$* and if $s = 1$, we say R is *strongly semismooth*.

In terms of this theory, $\mathbb{S} \in \partial R(\boldsymbol{\sigma}_{\text{tr}})$ is the algorithmically consistent tangent. This defines the standard solution method in computational plasticity, cf. Table 1.

(GN0)	Choose $\mathbf{u}_h^0 \in \mathbf{X}_h(\mathbf{u}_D)$, $\epsilon \geq 0$, and set $k := 1$.
(GN1)	Compute $\boldsymbol{\sigma}_{\text{tr}}^{k-1} = \mathbb{C}[\boldsymbol{\varepsilon}(\mathbf{u}_h^{k-1}) - \boldsymbol{\varepsilon}_p^{\text{old}}]$, the stress response $\boldsymbol{\sigma}^{k-1} = R(\boldsymbol{\sigma}_{\text{tr}}^{k-1})$, and the residual $r_{k-1}(\mathbf{w}_h) = \int_{\Omega} \boldsymbol{\sigma}^{k-1} : \boldsymbol{\varepsilon}(\mathbf{w}_h) dx - \ell(\mathbf{w}_h), \quad \mathbf{w}_h \in \mathbf{X}_h.$ If $\ r_{k-1}\ \leq \epsilon$, set $\mathbf{u}_h^* = \mathbf{u}_h^{k-1}$, STOP.
(GN2)	Choose $\mathbb{S} \in \partial R(\boldsymbol{\sigma}_{\text{tr}}^{k-1})$ and compute $\delta \mathbf{u}_h^k \in \mathbf{X}_h$ solving the linearized problem $\int_{\Omega} \mathbb{S}[\boldsymbol{\varepsilon}(\delta \mathbf{u}_h^k)] : \boldsymbol{\varepsilon}(\mathbf{w}_h) dx = -r_{k-1}(\mathbf{w}_h), \quad \mathbf{w}_h \in \mathbf{X}_h.$
(GN4)	Set $\mathbf{u}_h^k = \mathbf{u}_h^{k-1} + \delta \mathbf{u}_h^k$ and $k := k + 1$. Go to (GN1).

Table 1: Generic generalized Newton algorithm (GN) for one incremental step in elasto-plasticity.

Remark 3.1. *The algorithm (GN) requires a suitable initial iterate \mathbf{u}_h^0 ; otherwise, a damping strategy is required in order to obtain global convergence. On the other hand, using small time increments, a good initial iterate is usually available, and in most cases a quasi-static simulation with small increments is more efficient than a time consuming globalization strategy for the Newton method.*

Theorem 3.2. *Assume that there exists a solution \mathbf{u}_h^* to problem (2.15) and that R is semismooth (of order s), i.e. (3.1) holds. Moreover, we assume that for each choice*

$$\mathbb{S} \in \partial R(\mathbb{C}[\boldsymbol{\varepsilon}(\mathbf{u}_h^*) - \boldsymbol{\varepsilon}_p^{\text{old}}])$$

the bilinear form

$$(\mathbf{v}_h, \mathbf{w}_h) \mapsto \int_{\Omega} \mathbb{S}[\boldsymbol{\varepsilon}(\mathbf{v}_h)] : \boldsymbol{\varepsilon}(\mathbf{w}_h) dx$$

is non-singular. Then, the generalized Newton method (GN) in Table 1 converges locally superlinearly (of order $1 + s$).

For the *proof* we introduce a finite element basis $\boldsymbol{\psi}_1, \dots, \boldsymbol{\psi}_N$ of X_h , and we replace the integrals by a suitable quadrature. Then, the nonlinear variational problem (2.15) can be written as $F(y) = 0$ with a nonlinear function $F: \mathbb{R}^N \rightarrow \mathbb{R}^N$. Let y^* be the coefficient vector of the finite element solution \mathbf{u}_h^* . The choice of \mathbb{S} (at every integration point) defines the matrix

$$G(y^*) = \left(\int_{\Omega} \mathbb{S}[\boldsymbol{\varepsilon}(\boldsymbol{\psi}_i)] : \boldsymbol{\varepsilon}(\boldsymbol{\psi}_j) dx \right)_{i,j=1,\dots,N}.$$

Since the response function is the only nonlinear component in the construction of F , we can apply the chain rule Prop. A.3, i.e., F is also semismooth. Moreover, $G(y^*) \in \partial F(y^*)$. Thus, we can apply Prop. A.5, which gives the result.

Remark 3.3. *Although F is semismooth whenever the response function is semismooth, we cannot conclude in general, that $G(x^*) \in \partial F(x^*)$ is non-singular whenever \mathbb{S} is regular at every material point. This only holds for associated models with strict convex energies (where \mathbb{S} is symmetric positive definite), but for non-associated models, the global regularity has to be assumed additionally.*

3.1. Local evaluation of the response function

The response function \mathcal{R} is defined implicitly by the incremental flow rule (2.7), the evolution or state equation for the internal variables, and the complementarity conditions (2.9). The response depends on the trial stress $\boldsymbol{\sigma}_{\text{tr}}$ (which in fact is the input parameter of the algorithm) and the material history of the old time step $\boldsymbol{\eta}^{\text{old}}$ (which is fixed).

To evaluate the response function, we determine simultaneously the generalized stress $\boldsymbol{\Sigma} = (\boldsymbol{\sigma}, \boldsymbol{\eta}) \in \mathcal{S}$ and the consistency parameter $\Delta\lambda \in \mathbb{R}^p$. Thus, we define the space $\mathcal{T} = \mathcal{S} \times \mathbb{R}^p$, and we assume that a function $G: \mathcal{T} \times S \rightarrow \mathcal{S}$ exists, such that

$$G((\boldsymbol{\Sigma}, \Delta\lambda), \boldsymbol{\sigma}_{\text{tr}}) = 0 \quad (3.2)$$

holds if and only if the incremental flow rule (2.7) and the evolution or state equation for the internal variables are satisfied. The explicit construction of G depends on the application. E.g., for the hardening law in rate form as in (2.8), G takes the form

$$G(((\boldsymbol{\sigma}, \boldsymbol{\eta}), \Delta\lambda), \boldsymbol{\sigma}_{\text{tr}}) = \begin{bmatrix} \mathbb{C}^{-1}[\boldsymbol{\sigma} - \boldsymbol{\sigma}_{\text{tr}}] + \sum_{i=1}^p \Delta\lambda_i \mathbf{r}_i(\boldsymbol{\Sigma}) \\ \boldsymbol{\eta} - \boldsymbol{\eta}^{\text{old}} - \sum_{i=1}^p \Delta\lambda_i \mathbf{h}_i(\boldsymbol{\Sigma}) \end{bmatrix}.$$

To enforce the complementarity condition (2.9), we use an ncp-function¹ $\phi: \mathbb{R}^2 \rightarrow \mathbb{R}$ satisfying

$$\phi(f, \lambda) = 0 \quad \iff \quad f \leq 0, \quad \lambda \geq 0, \quad f\lambda = 0,$$

Then, the complementarity conditions are equivalent to

$$\Phi(f(\boldsymbol{\Sigma}), \Delta\lambda) = 0, \quad (3.3)$$

where the vector-valued npc-function $\Phi: \mathbb{R}^p \times \mathbb{R}^p \rightarrow \mathbb{R}^p$ is given by $\Phi_i(f, \lambda) = \phi(f_i, \lambda_i)$.

Here we use the ncp-function

$$\phi \equiv \phi_{\alpha}(f, \lambda) = \max\{0, \lambda + \alpha f\} - \lambda, \quad 0 < \alpha \in \mathbb{R}. \quad (3.4)$$

Note that ϕ is semismooth. An appropriate choice of the parameter $\alpha > 0$ may be important for the convergence properties of the active set method below. Of course, other ncp-functions can be used also.

Together, we now define the function

$$T: \mathcal{T} \times S \rightarrow \mathcal{T}, \quad T((\boldsymbol{\Sigma}, \Delta\lambda), \boldsymbol{\sigma}_{\text{tr}}) = \begin{bmatrix} G((\boldsymbol{\Sigma}, \Delta\lambda), \boldsymbol{\sigma}_{\text{tr}}) \\ \Phi(f(\boldsymbol{\Sigma}), \Delta\lambda) \end{bmatrix}, \quad (3.5)$$

which completely determines the plastic flow for a given trial stress $\boldsymbol{\sigma}_{\text{tr}} \in S$ (and given history variables of the previous time step): for a given trial stress $\boldsymbol{\sigma}_{\text{tr}}$, the solution $(\boldsymbol{\Sigma}^*, \Delta\lambda^*) \in K \times \mathbb{R}_{\geq 0}^p \subset \mathcal{T}$ of the nonlinear, nonsmooth equation

$$T((\boldsymbol{\Sigma}^*, \Delta\lambda^*), \boldsymbol{\sigma}_{\text{tr}}) = 0 \quad (3.6)$$

satisfies the equations for the material update. This implicit characterization is the basis for our analysis. For a precise formulation, we introduce the following notation for set-valued partial subdifferentials: $\mathbb{T} \in \partial_{(\boldsymbol{\Sigma}, \Delta\lambda)} T((\boldsymbol{\Sigma}, \Delta\lambda), \boldsymbol{\sigma}_{\text{tr}}) \subset \text{Lin}(\mathcal{T}, \mathcal{T})$ if and only if $\mathbb{P} \in \text{Lin}(S, \mathcal{T})$ exists such that $[\mathbb{T} \ \mathbb{P}] \in \partial T((\boldsymbol{\Sigma}, \Delta\lambda), \boldsymbol{\sigma}_{\text{tr}})$. Likewise, $\partial_{(\boldsymbol{\Sigma}, \Delta\lambda)}^B$ is defined.

Theorem 3.4. *Let T as given in (3.5) be semismooth (i.e. G and $\Phi(f(\cdot), \cdot)$ are semismooth) and for a given trial stress $\boldsymbol{\sigma}_{\text{tr}} \in S$ let $(\boldsymbol{\Sigma}^*, \Delta\lambda^*) \in \mathcal{T}$ be a solution of (3.6). Then, $(\boldsymbol{\Sigma}^*, \Delta\lambda^*) \in K \times \mathbb{R}_{\geq 0}^p$ is admissible. If in addition each element $\mathbb{T} \in \partial_{(\boldsymbol{\Sigma}, \Delta\lambda)} T((\boldsymbol{\Sigma}^*, \Delta\lambda^*), \boldsymbol{\sigma}_{\text{tr}})$ is non-singular, a neighborhood $U \subset S$ of $\boldsymbol{\sigma}_{\text{tr}}$ and a semismooth function $Y: U \subset S \rightarrow \mathcal{T}$ exists satisfying $Y(\boldsymbol{\sigma}_{\text{tr}}) = (\boldsymbol{\Sigma}^*, \Delta\lambda^*)$ and*

$$T(Y(\boldsymbol{\theta}), \boldsymbol{\theta}) = 0, \quad \boldsymbol{\theta} \in U. \quad (3.7)$$

Moreover, if $[\mathbb{T} \ \mathbb{P}] \in \partial^B T(Y(\boldsymbol{\theta}), \boldsymbol{\theta})$, we have

$$-\mathbb{T}^{-1}\mathbb{P} \in \partial^B Y(\boldsymbol{\theta}) \subset \partial Y(\boldsymbol{\theta}). \quad (3.8)$$

The *proof* is a direct application of the implicit function theorem for semismooth functions Prop. A.4.

We have $Y(\boldsymbol{\sigma}_{\text{tr}}) = (\mathcal{R}(\boldsymbol{\sigma}_{\text{tr}}), \Delta\lambda^*) = (R(\boldsymbol{\sigma}_{\text{tr}}), H(\boldsymbol{\sigma}_{\text{tr}}), \Delta\lambda^*)$, i.e., the first component of Y is just the (incremental) stress response function with $\boldsymbol{\sigma}^* = R(\boldsymbol{\sigma}_{\text{tr}})$ as given in (2.10). Thus, the theorem shows that the response function R is semismooth.

3.2. Computing the response function - an active set method

Within the generalized Newton method (GN) the stress response is evaluated (independently in every integration point) again by a generalized Newton method solving the nonlinear equation (3.6). For simplicity, we assume that G is differentiable, and we use the semismooth ncp-function $\phi \equiv \phi_{\alpha}$ as in (3.4). Then, T is also semismooth, and in order to formulate the Newton method, a generalized derivative has to be computed.

This can be done by an active set method. For $(\boldsymbol{\Sigma}, \Delta\lambda) \in \mathcal{T}$, we define the active index set

$$\mathcal{A}(\boldsymbol{\Sigma}, \Delta\lambda) = \{i \in \{1, \dots, p\} : \Delta\lambda_i + \alpha f_i(\boldsymbol{\Sigma}) > 0\},$$

¹npc = nonlinear complementarity problem

and for a given iterate $(\Sigma^{k-1}, \Delta\lambda^{k-1}) \in \mathcal{T}$, we set $\mathcal{A}_k = \mathcal{A}(\Sigma^{k-1}, \Delta\lambda^{k-1})$ and $\mathcal{I}_k = \{1, \dots, p\} \setminus \mathcal{A}_k$. For a matrix $A \in \mathbb{R}^{p,q}$ with rows A_i and an index set $\mathcal{J} \subset \{1, \dots, p\}$, we define $A_{\mathcal{J}}$ row-wise via $(A_{\mathcal{J}})_i = A_i$ if $i \in \mathcal{J}$ and $(A_{\mathcal{J}})_i = 0$ otherwise. This allows for a specific choice $\mathbb{T}((\Sigma, \Delta\lambda), \sigma_{\text{tr}}) \in \partial_{(\Sigma, \Delta\lambda)}^B T((\Sigma, \Delta\lambda), \sigma_{\text{tr}})$ defined by

$$\mathbb{T}((\Sigma, \Delta\lambda), \sigma_{\text{tr}}) := \begin{bmatrix} D_{\Sigma}G((\Sigma, \Delta\lambda), \sigma_{\text{tr}}) & D_{\Delta\lambda}G((\Sigma, \Delta\lambda), \sigma_{\text{tr}}) \\ \alpha Df(\Sigma)_{\mathcal{A}(\Sigma, \Delta\lambda)} & -\text{id}_{\mathcal{I}(\Sigma, \Delta\lambda)} \end{bmatrix},$$

Then, the corresponding generalized Newton method is equivalent to the (local) active set method (AS) which is given in Table 2.

-
- (AS0) Choose $(\Sigma^0, \Delta\lambda^0) \in \mathcal{T}$, $\epsilon \geq 0$, $\alpha > 0$ and set $k := 1$.
- (AS1) If $|T((\Sigma^{k-1}, \Delta\lambda^{k-1}), \sigma_{\text{tr}})| \leq \epsilon$,
set $(\Sigma^*, \Delta\lambda^*) = (\Sigma^{k-1}, \Delta\lambda^{k-1})$ and $\mathbb{T}^* = \mathbb{T}^{k-1}$, STOP.
- (AS2) Determine the active/inactive sets \mathcal{A}_k and \mathcal{I}_k and set $\mathbb{T}^k = \mathbb{T}((\Sigma^{k-1}, \Delta\lambda^{k-1}), \sigma_{\text{tr}})$.
- (AS3) Solve $\mathbb{T}^k[\delta\Sigma^k, \delta\Delta\lambda^k] = -T((\Sigma^{k-1}, \Delta\lambda^{k-1}), \sigma_{\text{tr}})$.
- (AS4) Set $(\Sigma^k, \Delta\lambda^k) = (\Sigma^{k-1}, \Delta\lambda^{k-1}) + (\delta\Sigma^k, \delta\Delta\lambda^k)$.
Set $k := k + 1$ and go to (AS1).
-

Table 2: Local active set method (AS) to determine the response function and the consistent tangent for a given trial stress σ_{tr} .

Again we can apply Prop. A.5: Since ϕ_{α} is semismooth and provided that f and G are differentiable, the algorithm (AS) converges superlinearly (quadratic if Df and DG are Lipschitz), if each element in $\partial_{(\Sigma, \Delta\lambda)} T((\Sigma^*, \Delta\lambda^*), \sigma_{\text{tr}})$ is non-singular and the initial guess is close to the solution.

Remark 3.5. In multi-yield plasticity, a suitable constraint qualification is required in order to guarantee that \mathbb{T}^k is regular. In some cases (e.g. for single crystal plasticity with many slip systems), $Df(\Sigma^{k-1})$ does not have full rank, so that \mathbb{T}^k is singular. In this case, the local active set method cannot be applied and has to be replaced by other solution methods.

3.3. Computation of the consistent tangent

For fast convergence of the (outer) generalized Newton method (GN), we need a suitable candidate for a generalized derivative $\mathbb{S} \in \partial R(\sigma_{\text{tr}})$ of the response function. Using $Y(\sigma_{\text{tr}}) = (\Sigma^*, \Delta\lambda^*) = (R(\sigma_{\text{tr}}), H(\sigma_{\text{tr}}), \Delta\lambda^*)$, Theorem 3.4 directly yields

$$\begin{bmatrix} \mathbb{S} \\ \mathbb{E} \\ \Lambda \end{bmatrix} := -(\mathbb{T}^*)^{-1} \mathbb{P}^* \in \partial Y(\sigma_{\text{tr}}) \quad (3.9)$$

for any choice $[\mathbb{T}^* \ \mathbb{P}^*] \in \partial^B T((\Sigma^*, \Delta\lambda^*), \sigma_{\text{tr}})$. If G and f are differentiable, we obtain \mathbb{T}^* directly in (AS) as the last generalized Jacobian in the response computation. In many applications, $\mathbb{P}^* \in \partial_{\sigma_{\text{tr}}} T((\Sigma^*, \Delta\lambda^*), \sigma_{\text{tr}})$ is easy to compute (often, it is linear with respect to σ_{tr}).

4. General associated plasticity with kinematic hardening

In our first example, we consider associated multi-yield plasticity with general linear kinematic hardening. It is well known that for vanishing hardening the perfectly plastic limit is obtained. Algorithmically, this corresponds to the closest point projection Simo et al. (1988a), and when applied to simple von Mises plasticity, this reduces to the classical radial return of Wilkins (1964).

We formally introduce the back-stress $\eta \in S$ and a corresponding conjugate interval variable $\delta \in S$ which are related by the state equation $\eta = -\mathbb{H}[\delta]$ with a symmetric positive semi-definite fourth order tensor $\mathbb{H} \in \text{Lin}(S, S)$. We consider the generalized stress space $K = \{(\sigma, \eta) \in S \times S : f(\sigma + \eta) \leq 0\}$. The associated flow rule follows by postulating maximal plastic dissipation, i.e. the flow rule is determined by maximizing $\sigma : \dot{\epsilon}_p + \eta : \dot{\delta}$ subject to $(\sigma, \eta) \in K$. Then

$$\dot{\epsilon}_p = \sum_{i=1}^p \lambda_i Df_i(\sigma + \eta) \quad \text{and} \quad \dot{\delta} = \sum_{i=1}^p \lambda_i Df_i(\sigma + \eta),$$

allowing to conclude $\epsilon_p = \delta$ if the initial conditions coincide, i.e. $\epsilon_p(0) = \delta(0)$. This leads to the incremental flow rule

$$\epsilon_p = \epsilon_p^{\text{old}} + \sum_{i=1}^p \Delta\lambda_i Df_i(\sigma + \eta) = \epsilon_p^{\text{old}} + \sum_{i=1}^p \Delta\lambda_i Df_i(\sigma - \mathbb{H}[\epsilon_p]).$$

For convenience, we define the relative stress $\alpha = \sigma + \eta = \sigma - \mathbb{H}[\epsilon_p]$ which allows us to conclude that plastic flow is determined by the system

$$\begin{aligned} \alpha &= \mathbb{C}[\epsilon(\mathbf{u}) - \epsilon_p^{\text{old}} - \sum_{i=1}^p \Delta\lambda_i Df_i(\alpha)] - \mathbb{H}[\epsilon_p] \\ &= \widehat{\sigma}_{\text{tr}} - \sum_{i=1}^p \Delta\lambda_i (\mathbb{C} + \mathbb{H})[Df_i(\alpha)], \\ 0 &= \Delta\lambda_i f_i(\alpha), \quad \Delta\lambda_i \geq 0, \quad f_i(\alpha) \leq 0. \end{aligned}$$

with $\widehat{\sigma}_{\text{tr}} = \sigma_{\text{tr}} - \mathbb{H}[\epsilon_p^{\text{old}}] = \mathbb{C}[\epsilon(\mathbf{u})] - (\mathbb{C} + \mathbb{H})[\epsilon_p^{\text{old}}]$. This yields $\alpha = P_K(\widehat{\sigma}_{\text{tr}})$ with the projection P_K w.r.t. the inner product induced by $\mathbb{N}^{-1} = (\mathbb{C} + \mathbb{H})^{-1}$. In terms of σ , this gives the incremental stress response

$$\sigma = (\mathbb{I} - \mathbb{C} \circ \mathbb{N}^{-1})[\widehat{\sigma}_{\text{tr}}] + \mathbb{C} \circ \mathbb{N}^{-1}[P_K(\widehat{\sigma}_{\text{tr}})] + \mathbb{H}[\epsilon_p^{\text{old}}].$$

Remark 4.1. In the simple case $\mathbb{H} = H_0 \mathbb{C}$ with $H_0 \geq 0$ we have $\mathbb{C} + \mathbb{H} = (1 + H_0)\mathbb{C}$, and P_K is the projection w.r.t. \mathbb{C}^{-1} and consequently

$$\sigma = \frac{H_0}{1+H_0} \widehat{\sigma}_{\text{tr}} + \frac{1}{1+H_0} P_K(\widehat{\sigma}_{\text{tr}}) + H_0 \mathbb{C}[\epsilon_p^{\text{old}}].$$

This includes the model of perfect plasticity ($H_0 = 0$), where $\sigma = P_K(\sigma_{\text{tr}})$.

The stress response function R has the same smoothness properties as the projection onto the admissible set. According to Section A.4, the projection is semismooth under quite general conditions.

Theorem 4.2. Suppose that $f_i \in C^2(S, \mathbb{R})$, $i = 1, \dots, p$ are convex and let $I(\boldsymbol{\eta}) = \{i \in \{1, \dots, p\} : f_i(\boldsymbol{\eta}) = 0\}$ be the set of active indices for given $\boldsymbol{\eta} \in S$. If $Df(\boldsymbol{\eta})_{I(\boldsymbol{\eta})}$ has rank $|I(\boldsymbol{\eta})|$ for all $\boldsymbol{\eta} \in \partial K$, then the response functions of perfect plasticity and linear kinematic hardening plasticity are semismooth.

Proof. The linear independence of the active indices implies the constant rank constrain qualification (CRCQ). Thus, as $f \in C^2(S, \mathbb{R})$, all orthogonal projections P_K are semismooth (Proposition A.6). \square

5. Von Mises/ J_2 plasticity with nonlinear hardening

To accomodate for strain hardening, an often used isotropic hardening law was proposed in Voce (1955), also see (Simo and Hughes, 1998, Section 3.3). As internal variable, we can use the accumulated plastic strain $e_p(t) = \int_0^t |\dot{\boldsymbol{\epsilon}}_p(s)| ds \geq 0$. Via the potential

$$\Psi_v(e_p) = \frac{1}{2}H_0e_p^2 + (K_\infty - K_0)(e_p + \frac{1}{\delta} \exp(-\delta e_p)),$$

we can also express hardening in terms of the conjugate stress

$$\eta = D\Psi_v(e_p) = H_0e_p + (K_\infty - K_0)(1 - \exp(-\delta e_p)) \geq 0,$$

with material constants $H_0 \geq 0$ (linear hardening modulus), $K_\infty \geq K_0 \geq 0$ (saturation constants) and $\delta > 0$ (saturation growth constant). Particularly, for $K_\infty = K_0$ and $H_0 > 0$, we obtain linear isotropic hardening. For the generalized stress $\Sigma = (\boldsymbol{\sigma}, \eta) \in S \times \mathbb{R}$ we consider the yield function

$$f(\boldsymbol{\sigma}, \eta) = |\text{dev}(\boldsymbol{\sigma})| - \eta - Y_0.$$

In terms of e_p , this is sometimes written as $f(\boldsymbol{\sigma}, e_p) = |\text{dev}(\boldsymbol{\sigma})| - Y(e_p)$ with the dissipation function $Y(e_p) = Y_0 + H_0e_p + (K_\infty - K_0)(1 - \exp(-\delta e_p))$, cf. Gurtin and Reddy (2009). Based on the the principle of maximum plastic dissipation, i.e.

$$\max \quad \boldsymbol{\sigma} : \dot{\boldsymbol{\epsilon}}_p - \eta \dot{e}_p \quad \text{subject to} \quad f(\boldsymbol{\sigma}, \eta) \leq 0, \eta \geq 0,$$

we obtain the associated flow rule

$$\dot{\boldsymbol{\epsilon}}_p = \lambda D\boldsymbol{\sigma}f(\boldsymbol{\sigma}, \eta) = \lambda \frac{\text{dev}(\boldsymbol{\sigma})}{|\text{dev}(\boldsymbol{\sigma})|}, \quad \text{and} \quad \dot{e}_p = \lambda, \quad (5.1)$$

as the corresponding optimality condition (please note that the additional Lagrange multiplier corresponding to $\eta \geq 0$ vanishes). We also remark that then $|\dot{\boldsymbol{\epsilon}}_p| = \lambda = \dot{e}_p \geq 0$ justifying the definition of the accumulated plastic strain above.

In the incremental problem, it is well known that the flow direction can be obtained from the trial stress directly as $\boldsymbol{n} = \frac{\text{dev}(\boldsymbol{\sigma})}{|\text{dev}(\boldsymbol{\sigma})|} = \frac{\text{dev}(\boldsymbol{\sigma}_{\text{tr}})}{|\text{dev}(\boldsymbol{\sigma}_{\text{tr}})|}$, and we find

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_{\text{tr}} - \Delta\lambda\mathbb{C}[\boldsymbol{n}] \quad \text{and} \quad \eta = D\Psi_v(e_p) = D\Psi_v(e_p^{\text{old}} + \Delta\lambda).$$

Following the framework of Section 3.1, we define

$$G((\boldsymbol{\sigma}, \eta), \Delta\lambda, \boldsymbol{\sigma}_{\text{tr}}) = \begin{bmatrix} \boldsymbol{\sigma} - \boldsymbol{\sigma}_{\text{tr}} + \Delta\lambda\mathbb{C}[\boldsymbol{n}] \\ \eta - D\Psi_v(e_p^{\text{old}} + \Delta\lambda) \end{bmatrix}$$

and perform the active set method. However, as this is a single-yield model, the solution of equation (3.6) and thus the stress response can be determined easily. If $f(\boldsymbol{\sigma}_{\text{tr}}, \eta^{\text{old}}) \leq 0$, we can set $\boldsymbol{\sigma} = \boldsymbol{\sigma}_{\text{tr}}$, $\Delta\lambda = 0$ and $e_p = e_p^{\text{old}}$. Otherwise, we require $f(\boldsymbol{\sigma}, \eta) = 0$ and $G((\boldsymbol{\sigma}, \eta), \Delta\lambda) = 0$. This can be reduced to a scalar nonlinear equation $h(\Delta\lambda) = 0$ for the consistency parameter as

$$0 = f(\boldsymbol{\sigma}, \eta) = f(\boldsymbol{\sigma}_{\text{tr}} - \Delta\lambda\mathbb{C}[\boldsymbol{n}], D\Psi_v(e_p^{\text{old}} + \Delta\lambda)) =: h(\Delta\lambda).$$

Via implicit differentiation, the corresponding consistent tangent can be determined explicitly, cf. (Simo and Hughes, 1998, Section 3.3). Nevertheless, concerning semismoothness of the response function, the representation via $T(((\boldsymbol{\sigma}, \eta), \Delta\lambda), \boldsymbol{\sigma}_{\text{tr}})$ is more adequate.

Theorem 5.1. For any given $\boldsymbol{\sigma}_{\text{tr}} \in S$ and $e_p^{\text{old}} \geq 0$, the response function $R(\boldsymbol{\sigma}_{\text{tr}})$ is semismooth.

Proof. The existence of a unique solution can easily be checked, cf. (Simo and Hughes, 1998, Section 3.3). At a solution $\Sigma^* = (\boldsymbol{\sigma}^*, \eta^*)$ we always find that G is differentiable and we conclude that T is semismooth by using the semismooth ncp-function (3.4). By the implicit function theorem for semismooth functions (Proposition A.4), this also shows the semismoothness of the response function, since it can be shown that T^* is always regular. \square

6. Drucker-Prager plasticity

A basic and widely used model in soil plasticity is the (non-associated) Drucker-Prager model. For simplicity, we only consider perfect plasticity and $d = 3$. A specific feature of the Drucker-Prager model is the non-differentiability of the yield function at the boundary of the elastic domain. This is often seen as a drawback and we also consider a smoothed variant (Krabbenhoft et al., 2006; Miehe and Lambrecht, 1999), which renders the yield function smooth at the expense that it is no longer possible to write down the response function explicitly.

6.1. Classical Drucker-Prager plasticity

The yield function

$$f(\boldsymbol{\sigma}) = |\text{dev}(\boldsymbol{\sigma})| + k_0(\tan \phi \frac{1}{3} \text{tr}(\boldsymbol{\sigma}) - c)$$

defines the admissible set K , which is a cone with apex $\boldsymbol{\sigma}_{\text{apex}} = \frac{c}{\tan \phi} \mathbf{1}$. It is important to note that f is not differentiable at the apex of the cone. Here, $k_0 > 0$ is a shape factor of the cone, $c \geq 0$ is related to the cohesion, and $\phi > 0$ is the angle of friction. The non-associated flow rule is based on the plastic potential

$$g(\boldsymbol{\sigma}) = |\text{dev}(\boldsymbol{\sigma})| + k_0(\tan \psi \frac{1}{3} \text{tr}(\boldsymbol{\sigma}) - c),$$

where $\psi \in [0, \phi]$ is the dilatency.

The incremental flow rule is then given as

$$\boldsymbol{\epsilon}_p = \boldsymbol{\epsilon}_p^{\text{old}} + \Delta\lambda \boldsymbol{s}, \quad \boldsymbol{s} \in \partial g(\boldsymbol{\sigma}),$$

where $s \in \partial g(\boldsymbol{\sigma})$ coincides with $Dg(\boldsymbol{\sigma})$ whenever g is differentiable at $\boldsymbol{\sigma}$, i.e. if $\text{dev}(\boldsymbol{\sigma}) \neq 0$. Defining

$$\mathbb{G}[\boldsymbol{\varepsilon}] = \text{dev}(\boldsymbol{\varepsilon}) + \frac{\tan \psi}{\tan \phi} \frac{1}{3} \text{tr}(\boldsymbol{\varepsilon}) \mathbf{1},$$

we find $\boldsymbol{\varepsilon}_p = \boldsymbol{\varepsilon}_p^{\text{old}} + \Delta \lambda \mathbb{G}[s]$, with $s \in \partial f(\boldsymbol{\sigma})$. If $\psi > 0$, \mathbb{G} is invertible and for isotropic materials we obtain

$$0 \in (\mathbb{C} \circ \mathbb{G})^{-1}[\boldsymbol{\sigma} - \boldsymbol{\sigma}_{\text{tr}}] + \Delta \lambda s, \quad s \in \partial f(\boldsymbol{\sigma}). \quad (6.1)$$

Together with the complementarity condition, we find $\boldsymbol{\sigma} = P_k^F(\boldsymbol{\sigma}_{\text{tr}})$ with P_k^F being the orthogonal projection onto the admissible set K w.r.t. the inner product induced by $\mathbb{F}^{-1} := (\mathbb{C} \circ \mathbb{G})^{-1}$.

Theorem 6.1. *If $\psi > 0$, the stress response function of classical Drucker-Prager plasticity is strongly semismooth.*

Proof. The admissible set admits a representation as a scaled and shifted second order unit cone, since

$$K = \left\{ \boldsymbol{\sigma} = (\text{dev } \boldsymbol{\sigma}, \frac{1}{d} \text{tr}(\boldsymbol{\sigma})) \in S_0 \times \mathbb{R} : |\text{dev}(\boldsymbol{\sigma})| \leq k_0(c - \tan \phi \frac{1}{3} \text{tr}(\boldsymbol{\sigma})) \right\}.$$

The response function is an orthogonal projection if $\psi > 0$ and by Proposition A.7, we find that R is strongly semismooth. \square

The response function can be given explicitly by means of the dual cone K° of K with respect to the inner product induced by $\mathbb{F}^{-1} = (\mathbb{C} \circ \mathbb{G})^{-1}$, i.e.,

$$K^\circ = \left\{ \boldsymbol{\sigma} \in S : \mathbb{F}^{-1}[\boldsymbol{\sigma}] : \boldsymbol{\theta} \leq 0 \text{ for all } \boldsymbol{\theta} \in K \right\}.$$

With $k^\circ(\boldsymbol{\sigma}) := \kappa \tan \phi \tan \psi |\text{dev}(\boldsymbol{\sigma})| - 2\mu \left(\frac{\tan \phi}{3} \text{tr}(\boldsymbol{\sigma}) - c \right)$, we obtain $K^\circ = \{ \boldsymbol{\sigma} \in S : k^\circ(\boldsymbol{\sigma}) \leq 0 \}$ and the projection/response $R(\boldsymbol{\sigma}_{\text{tr}}) = P_K^F(\boldsymbol{\sigma}_{\text{tr}})$ is given as

$$P_K^F(\boldsymbol{\sigma}_{\text{tr}}) = \begin{cases} \boldsymbol{\sigma}_{\text{tr}} & f(\boldsymbol{\sigma}_{\text{tr}}) \leq 0, \\ \boldsymbol{\sigma}_{\text{apex}} & k^\circ(\boldsymbol{\sigma}_{\text{tr}}) \leq 0, \\ \boldsymbol{\sigma}_{\text{tr}} - \frac{f(\boldsymbol{\sigma}_{\text{tr}})}{2\mu + \tan \phi \tan \psi \kappa} \mathbb{F}[Df(\boldsymbol{\sigma}_{\text{tr}})] & \text{else.} \end{cases}$$

In the latter case $Df(\boldsymbol{\sigma}_{\text{tr}}) = (2\mu \frac{\text{dev}(\boldsymbol{\sigma}_{\text{tr}})}{|\text{dev}(\boldsymbol{\sigma}_{\text{tr}})} + \kappa \tan \phi \mathbf{1})$ exists since $\boldsymbol{\sigma}_{\text{tr}} \notin K \cup K^\circ$ implies $\text{dev}(\boldsymbol{\sigma}_{\text{tr}}) \neq 0$. Moreover, in this case we can define

$$\mathbb{S}_{\text{reg}}(\boldsymbol{\sigma}_{\text{tr}}) := \mathbb{I} - \frac{1}{2\mu + \kappa \tan \phi \tan \psi} \left(\mathbb{F}[Df(\boldsymbol{\sigma}_{\text{tr}})] \otimes Df(\boldsymbol{\sigma}_{\text{tr}}) + f(\boldsymbol{\sigma}_{\text{tr}}) \mathbb{F} \circ D^2 f(\boldsymbol{\sigma}_{\text{tr}}) \right),$$

with $D^2 f(\boldsymbol{\sigma}_{\text{tr}})[\boldsymbol{\varepsilon}] = \frac{1}{|\text{dev}(\boldsymbol{\sigma}_{\text{tr}})} \left(\text{dev}(\boldsymbol{\varepsilon}) - \frac{\text{dev}(\boldsymbol{\sigma}_{\text{tr}}) : \boldsymbol{\varepsilon}}{|\text{dev}(\boldsymbol{\sigma}_{\text{tr}})} \frac{\text{dev}(\boldsymbol{\sigma}_{\text{tr}})}{|\text{dev}(\boldsymbol{\sigma}_{\text{tr}})} \right)$. Eventually, setting

$$\mathbb{S} \equiv \mathbb{S}(\boldsymbol{\sigma}_{\text{tr}}) = \begin{cases} \mathbb{I} & f(\boldsymbol{\sigma}_{\text{tr}}) \leq 0, \\ 0 & k^\circ(\boldsymbol{\sigma}_{\text{tr}}) \leq 0, \\ \mathbb{S}_{\text{reg}}(\boldsymbol{\sigma}_{\text{tr}}) & \text{else,} \end{cases}$$

we find $\mathbb{S} \in \partial P_K^F(\boldsymbol{\sigma}_{\text{tr}})$ as the algorithmically consistent tangent. More details can be found in Sauter (2010, Section 7.4.2).

6.2. Smoothed Drucker-Prager plasticity

Since f is not differentiable, we also consider a smoothed variant, cf. Krabbenhoft et al. (2006); Miehe and Lambrecht (1999). For a smoothing parameter $\theta > 0$, we define

$$f_\theta(\boldsymbol{\sigma}) = \sqrt{|\text{dev}(\boldsymbol{\sigma})|^2 + \theta^2} + k_0(\tan \phi \frac{1}{3} \text{tr}(\boldsymbol{\sigma}) - c),$$

$$g_\theta(\boldsymbol{\sigma}) = \sqrt{|\text{dev}(\boldsymbol{\sigma})|^2 + \theta^2} + k_0(\tan \psi \frac{1}{3} \text{tr}(\boldsymbol{\sigma}) - c).$$

and enforce $0 = G(\boldsymbol{\sigma}, \Delta \lambda) = \mathbb{C}^{-1}[\boldsymbol{\sigma} - \boldsymbol{\sigma}_{\text{tr}}] + \Delta \lambda Dg_\theta(\boldsymbol{\sigma})$ instead of (6.1).

Theorem 6.2. *If $\psi > 0$, the stress response is uniquely defined and the response function is semismooth.*

Proof. By the same arguments as above, the response function can be interpreted as the orthogonal projection w.r.t. $(\mathbb{C} \circ \mathbb{G})^{-1}$ and the result follows from Proposition A.6. Alternatively, we can apply Theorem 3.4. \square

For smoothed Drucker-Prager plasticity, we will shortly indicate that the consistent tangent \mathbb{S} as introduced in Section 3.3 does indeed coincide with the definition given in Simo and Taylor (1985); Simo and Hughes (1998). In this simple single-yield model, we have $p = 1$ and the active set at the solution is trivially given by

$$\mathcal{A}^* = \begin{cases} \{1\} & \Delta \lambda^* + \alpha f(\boldsymbol{\sigma}^*) > 0, \\ \emptyset & \Delta \lambda^* + \alpha f(\boldsymbol{\sigma}^*) \leq 0. \end{cases}$$

Since at the same time, the solution fulfills the complementarity conditions (2.9) and in particular $f(\boldsymbol{\sigma}^*) \leq 0$, we find that in the second case we have $\Delta \lambda^* = 0$ and the response is elastic, i.e. $\boldsymbol{\sigma} = \boldsymbol{\sigma}_{\text{tr}}$. Otherwise, we observe $\Delta \lambda^* > 0$ and necessarily $f(\boldsymbol{\sigma}^*) = 0$ and $\boldsymbol{\sigma}_{\text{tr}} \notin K$. This gives

$$\mathbb{T}^* = \begin{bmatrix} \mathbb{C}^{-1} + \Delta \lambda^* D^2 g_\theta(\boldsymbol{\sigma}^*) & Dg_\theta(\boldsymbol{\sigma}^*)^T \\ \alpha Df_\theta(\boldsymbol{\sigma}^*) & 0 \end{bmatrix} \quad \text{and} \quad \mathbb{P}^* = \begin{bmatrix} -\mathbb{C}^{-1} \\ 0 \end{bmatrix},$$

cf. (3.9). We set $\mathbb{A} = (\mathbb{C}^{-1} + \Delta \lambda^* D^2 g_\theta(\boldsymbol{\sigma}^*))^{-1}$ (note that this is the exact Hessian matrix Ξ in Simo and Hughes (1998, Chap. 3.6.1)) and the inverse of \mathbb{T}^* is

$$\begin{bmatrix} \mathbb{A} - \frac{\mathbb{A}[Dg_\theta(\boldsymbol{\sigma}^*)] \otimes \mathbb{A}[Df_\theta(\boldsymbol{\sigma}^*)]}{Df_\theta(\boldsymbol{\sigma}^*) : \mathbb{A}[Dg_\theta(\boldsymbol{\sigma}^*)]} & \frac{\mathbb{A}[Dg_\theta(\boldsymbol{\sigma}^*)]}{\alpha Df_\theta(\boldsymbol{\sigma}^*) : \mathbb{A}[Dg_\theta(\boldsymbol{\sigma}^*)]} \\ \frac{\mathbb{A}[Df_\theta(\boldsymbol{\sigma}^*)]}{Df_\theta(\boldsymbol{\sigma}^*) : \mathbb{A}[Dg_\theta(\boldsymbol{\sigma}^*)]} & \frac{-1}{\alpha Df_\theta(\boldsymbol{\sigma}^*) : \mathbb{A}[Dg_\theta(\boldsymbol{\sigma}^*)]} \end{bmatrix}.$$

According to (3.9), this gives the consistent tangent as

$$\mathbb{S} = \left(\mathbb{A} - \frac{\mathbb{A}[Dg_\theta(\boldsymbol{\sigma}^*)] \otimes \mathbb{A}[Df_\theta(\boldsymbol{\sigma}^*)]}{Df_\theta(\boldsymbol{\sigma}^*) : \mathbb{A}[Dg_\theta(\boldsymbol{\sigma}^*)]} \right) \circ \mathbb{C}^{-1}.$$

We see that in the simple case of single-yield plasticity, the approach of Section 3 reduces to the well-known formulas for the algorithmically consistent tangent.

7. Modified Cam-clay plasticity

Cam-clay plasticity and its variants (Roscoe and Burland, 1968; Roscoe and Wroth, 1968) are fundamental models in critical state soil mechanics in which pressure sensitivity plays a dominant role in the sense that depending on the mean stress, the materials may exhibit hardening or softening behaviour. Modified Cam-clay is an enhancement of the original Cam-clay model, and, in contrast to its predecessor, has a smooth yield surface, being an ellipse in the deviatoric-hydrostatic plane. We mainly follow the presentation given in Borja and Lee (1990) and Zouain et al. (2007). In the former, also a return algorithm in order to compute the response function and the consistent tangent is given. Yet, being a key model in soil mechanics, analytical results concerning existence and uniqueness of the underlying initial boundary value problem have only been obtained recently, cf. Dal Maso and DeSimone (2009); Dal Maso et al. (2011). A main feature is that the yield function is not convex w.r.t. the generalized stress $\Sigma = (\sigma, \eta) \in S \times \mathbb{R}$ and that the hardening law is non-associated. The material strength parameter $\eta > 0$ (related to the pre-consolidation pressure) serves as an internal variable and determines the radius of the ellipse in the direction of the hydrostatic pressure axis. For the ease of notation, we use the abbreviations

$$q = \sqrt{\frac{3}{2}} |\text{dev}(\sigma)| \quad \text{and} \quad p = -\sigma_m = -\frac{1}{3} \text{tr}(\sigma),$$

with the mean stress σ_m , where by convention the compression is negative. The yield function is given as

$$\begin{aligned} f(\Sigma) &= f(\sigma, \eta) = f(q, p, \eta) = q^2 - M^2 p(2\eta - p) \\ &= \frac{3}{2} |\text{dev}(\sigma)|^2 + M^2 \sigma_m (\sigma_m + 2\eta). \end{aligned}$$

Concerning the plastic strain rate we assume normality (however, also non-associated flow directions are possible as in Borja and Lee (1990)), but for the evolution of the strength parameter, a non-associated evolution law is proposed, i.e.

$$\dot{\epsilon}_p = \lambda D_{\sigma} f(\sigma, \eta),$$

$$\dot{\eta} = -k\eta \text{tr}(\dot{\epsilon}_p) = -k\eta \lambda D_{\sigma_m} f(\sigma, \eta) = -2M^2 k\eta \lambda (\sigma_m + \eta),$$

with the material parameter k related to the virgin compression and the swell-recompression index. Concerning the evolution law for the internal variable η , there are two possibilities: either we use our standard approach and approximate time derivatives by backward differences, or we solve the differential equation exactly in terms of the plastic strain rate which gives

$$\eta = \eta^{\text{old}} \exp(-k(\text{tr}(\epsilon_p) - \text{tr}(\epsilon_p^{\text{old}}))). \quad (7.1)$$

The exact integration allows to conclude that η always has the same sign as η^{old} . Contrary, using backward differences in the evolution law for η , this is not necessarily the case. Replacing the evolution equation for η by the state equation (7.1) gives

$$G((\sigma, \eta), \Delta\lambda, \sigma_{\text{tr}}) = \left[\begin{array}{c} \mathbb{C}^{-1}[\sigma - \sigma_{\text{tr}}] + \Delta\lambda D_{\sigma} f(\sigma, \eta) \\ \eta - \eta^{\text{old}} \exp(k \text{tr}(\mathbb{C}^{-1}[\sigma - \sigma_{\text{tr}}])) \end{array} \right].$$

Here, the incremental evolution law for the internal variables does not take the form (2.8).

Following Theorem 3.4, we have:

Theorem 7.1. *Let ϵ_p^{old} and $\eta^{\text{old}} > 0$ be given, and assume that a unique solution $(\mathbf{u}^*, \sigma^*, \eta^*)$ of the incremental problem exists satisfying $T((\sigma^*, \eta^*), \Delta\lambda^*, \sigma_{\text{tr}}^*) = 0$ with $\sigma_{\text{tr}}^* = \mathbb{C}[\epsilon(\mathbf{u}^*) - \epsilon_p^{\text{old}}]$. Moreover, assume that all elements in $\partial_{(\sigma, \eta, \Delta\lambda)} T((\sigma^*, \eta^*), \Delta\lambda^*, \sigma_{\text{tr}}^*)$ are non-singular. Then, the stress response function R is semismooth.*

8. A (Drucker-Prager) cap model

Drucker-Prager plasticity as presented in Section 6 has the drawback that it allows infinitely large hydrostatic compression. Therefore, it has been proposed to cap the unbounded set of admissible states, cf. DiMaggio and Sandler (1971); Simo et al. (1988b); Hofstetter et al. (1993). So similarly to the Cam-clay model, the admissible set is bounded in the σ -space. However, instead of taking the form of an ellipse, the yield surface is composed of three parts ($p = 3$): a Drucker-Prager-like failure criterium, a tension cutoff and a bounding hardening/softening cap. The generalized stress again takes the form $\Sigma = (\sigma, \eta) \in S \times \mathbb{R}$, with η being a material strength parameter determining the center of the elliptic cap as given below by the yield function f_2 . Analytical results concerning the initial boundary value problem have only been obtained recently Babadjian et al. (2011). Setting

$$F_e(p) = C - \gamma_1 e^{-\gamma_2 p} + \theta p,$$

$$F_c(p, \eta) = \frac{1}{R^2} (X(\eta) - \max\{0, \eta\})^2 - (p - \max\{0, \eta\})^2,$$

the yield functions are given as

$$f_1(\Sigma) = f_1(q, p) = q - F_e(p) \quad (\text{linear-exponential DP})$$

$$f_2(\Sigma) = f_2(q, p, \eta) = q^2 - F_c(p, \eta)^2 \quad (\text{elliptic cap})$$

$$f_3(\Sigma) = f_3(p) = p - T \quad (\text{tension cutoff})$$

with the following material parameters: $\gamma_i \geq 0$ are shape parameters of the linear-exponential Drucker-Prager failure criterium, θ is related to the angle of friction, R is the shape parameter of the elliptic cap, and $T \geq 0$ the tension cutoff. We remark that only the elliptic cap described by f_2 depends on the strength parameter, but not the linear-exponential Drucker-Prager envelope and the tension cutoff.

The tension cutoff T must be chosen such that $T < p^*$, where p^* denotes the zero of $F_e(p) = 0$. If $\gamma_i = 0$, f_1 reduces to the Drucker-Prager criterium and $p^* = -\frac{C}{\theta}$, which is just the volumetric stress at the apex of the Drucker-Prager cone. If $T \geq p^*$, the tension cutoff would be redundant as $f_1(\Sigma) \leq 0$ would imply $f_3(\Sigma) \leq 0$. Hence, we always consider $T < p^*$. In this case, we can guarantee that if the yield condition i is active, f_i is differentiable at the corresponding stress state. We also remark that—as for the modified Cam-clay model— f_2 is not convex with respect to the strength parameter η since the cap is elliptic. In order to have convex yield functions, also parabolic (linear w.r.t. η , quadratic w.r.t. p) and linear caps have been proposed.

For the plastic flow direction, we again assume normality, i.e. $\dot{\boldsymbol{\varepsilon}}_p = \sum_{i=1}^3 \lambda_i Df_i(\boldsymbol{\sigma}, \eta)$ giving the incremental law

$$\boldsymbol{\varepsilon}_p = \boldsymbol{\varepsilon}_p^{\text{old}} + \sum_{i=1}^3 \Delta \lambda_i D\sigma f_i(\boldsymbol{\sigma}, \eta),$$

but again a non-associated hardening law is enforced. Various formulations have been proposed, e.g., the state law (DiMaggio and Sandler, 1971)

$$\text{tr}(\boldsymbol{\varepsilon}_p) = W(1 - e^{-DX(\eta)}). \quad (8.1)$$

Here, $X(\eta) = \eta + RF_e(\eta)$ denotes the intersection of the cap with the hydrostatic axis and D, W are material parameters. In terms of $\boldsymbol{\sigma}$ and $\boldsymbol{\sigma}_{\text{tr}}$, we then define

$$G((\boldsymbol{\sigma}, \eta), \Delta \lambda), \boldsymbol{\sigma}_{\text{tr}}) = \left[\begin{array}{c} \mathbb{C}^{-1}[\boldsymbol{\sigma} - \boldsymbol{\sigma}_{\text{tr}}] + \sum_{i=1}^3 \Delta \lambda_i D\sigma f_i(\boldsymbol{\sigma}, \eta) \\ \text{tr}(\mathbb{C}^{-1}[\boldsymbol{\sigma}_{\text{tr}} - \boldsymbol{\sigma} + \mathbb{C}[\boldsymbol{\varepsilon}_p^{\text{old}}]]) - W(1 - e^{-DX(\eta)}) \end{array} \right],$$

and the ncp-function

$$\Phi(f(\boldsymbol{\Sigma}), \Delta \lambda) = \left[\begin{array}{c} \phi(f_1(\boldsymbol{\sigma}), \Delta \lambda_1) \\ \phi(f_2(\boldsymbol{\sigma}, \eta), \Delta \lambda_2) \\ \phi(f_3(\boldsymbol{\sigma}), \Delta \lambda_3) \end{array} \right].$$

The resulting equation $T((\boldsymbol{\Sigma}, \Delta \lambda), \boldsymbol{\sigma}_{\text{tr}}) = 0$ is a nonsmooth equation in \mathbb{R}^{10} . Application of Theorem 3.4 gives the following result.

Theorem 8.1. *Assume that the incremental problem has a unique solution $(\boldsymbol{\varepsilon}(\mathbf{u}^*), \boldsymbol{\sigma}^*, \eta^*)$ satisfying $T((\boldsymbol{\sigma}^*, \eta^*), \Delta \lambda^*), \boldsymbol{\sigma}_{\text{tr}}^*) = 0$ with $\boldsymbol{\sigma}_{\text{tr}}^* = \mathbb{C}[\boldsymbol{\varepsilon}(\mathbf{u}^*) - \boldsymbol{\varepsilon}_p^{\text{old}}]$, and assume that all elements in $\partial_{(\boldsymbol{\sigma}, \eta, \Delta \lambda)} T((\boldsymbol{\sigma}^*, \eta^*), \Delta \lambda^*), \boldsymbol{\sigma}_{\text{tr}}^*)$ are non-singular. Then, the stress response function R is semismooth.*

9. Numerical examples - (smoothed) Drucker-Prager

All computations have been performed with the parallel finite element program M++ (Wieners, 2010), which provides a large class of linear solvers and preconditioners (including multigrid).

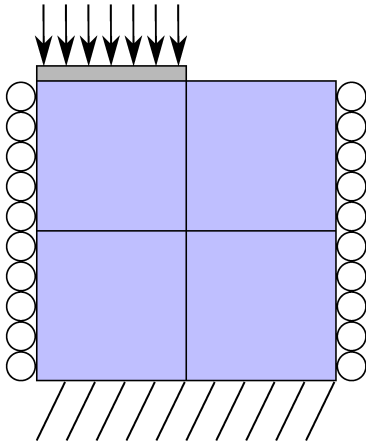


Figure 1: Geometry of the strip footing.

9.1. A strip footing

We apply the non-associated Drucker-Prager material models to a simple strip footing problem in 2D. Material parameters, the geometry and some computational details can be found in Table 3 and Figure 1. The smoothing parameter $\theta = 0.0001$ is very small such that the material response of the classical and the smoothed Drucker-Prager model are comparable. The load is applied with a constant rate in 60 incremental load steps and at the final time $T = 6$, over 90% of the specimen are plastified.

Material parameters		
Shear modulus:	μ	5.5 MPa
Bulk modulus:	κ	12.07 MPa
Cohesion:	c	0.01 MPa
Friction angle:	ϕ	30°
Dilatancy angle:	ψ	15°
Scaling factor:	k_0	0.7
Smoothing parameter:	θ	0.0001

Computational details		
Degrees of freedom:		132 098
Final time:	T	6
Time step size:	Δt	0.1

Table 3: Material parameters of the (smoothed) Drucker-Prager model, computational details and geometry of the strip footing.

Table 4 shows the nonlinear convergence history of the (outer) Newton method at the times $t_{20} = 2$ ($\approx 5\%$ plastification), $t_{40} = 4$ ($\approx 50\%$ plastification) and $t_{60} = T$ ($\approx 90\%$ plastification). The iteration was stopped if either the Euclidian norm of the residual was reduced by factor of $1e-08$ or was below $1e-10$. We clearly observe superlinear convergence for both models. While for Drucker-Prager, we could use the closed-form representation of the incremental response, for the smoothed variant, we performed the active set method proposed in Section 3.2 in order to compute the stress response and the consistent tangent.

k	Drucker-Prager			Smoothed Drucker-Prager		
	t_{20}	t_{40}	t_{60}	t_{20}	t_{40}	t_{60}
0	4.4e-05	8.2e-05	2.8e-04	4.4e-05	8.2e-05	2.8e-04
1	2.8e-05	8.3e-06	1.4e-04	4.4e-05	8.2e-06	1.4e-04
2	1.0e-05	4.4e-07	5.0e-06	2.8e-06	4.3e-07	5.1e-06
3	3.8e-07	1.5e-08	1.0e-06	9.5e-08	2.1e-08	1.0e-06
4	1.1e-08	4.6e-14	3.4e-07	1.8e-09	7.8e-14	3.3e-07
5	1.8e-14		1.5e-07	2.4e-15		1.5e-07
6			6.9e-08			5.9e-08
7			2.2e-08			1.1e-08
8			1.5e-11			4.7e-13

Table 4: Convergence history of the (outer) generalized Newton iteration for Drucker-Prager and smoothed Drucker-Prager elasto-plasticity.

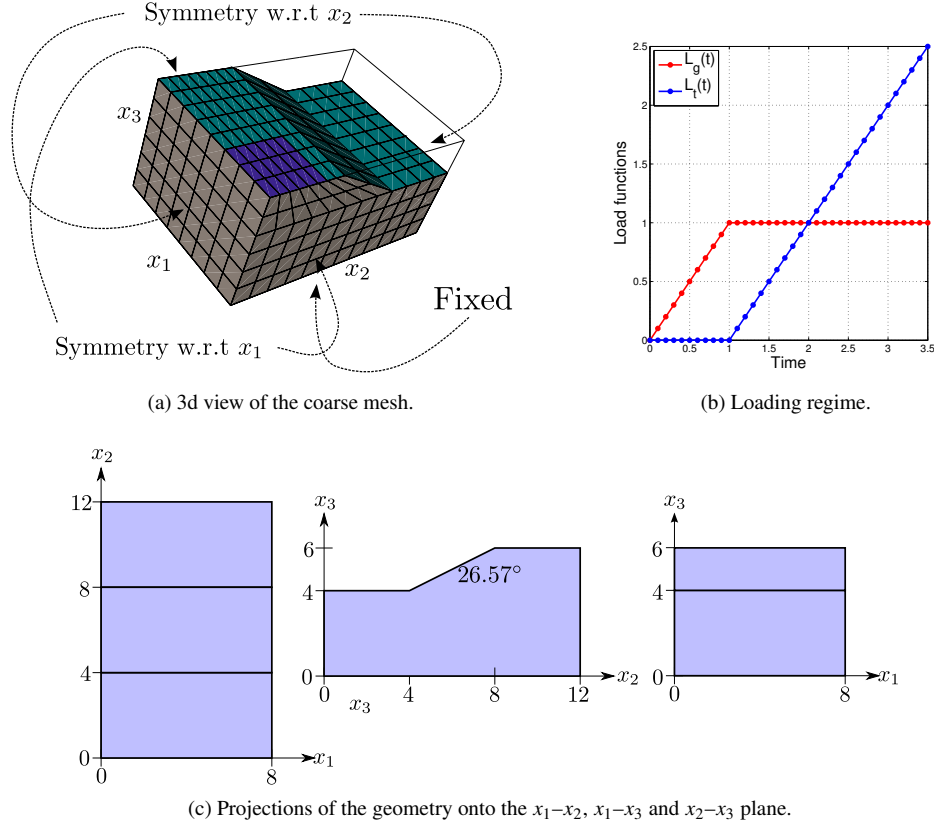


Figure 2: Geometry of the slope and the loading regime.

9.2. A slope failure problem

We now consider a more challenging 3d slope failure problem. The slope geometry and boundary conditions are shown in Figure 2. Again, we use the Drucker-Prager material model, but this time, we use the viscoplastic regularization of Duvaut-Lions (2.5) with parameter $\beta = 0.0005$. In the incremental setting, the flow rule becomes

$$\boldsymbol{\varepsilon}_p = \boldsymbol{\varepsilon}_p^{\text{old}} + \frac{\Delta t}{\beta} \mathbb{C}^{-1} [\boldsymbol{\sigma} - \bar{\boldsymbol{\sigma}}],$$

where $\bar{\boldsymbol{\sigma}}$ denotes the response of the rate-independent problem. Substitution in Hooke's law (2.2) then gives

$$\boldsymbol{\sigma} = \frac{\beta}{\beta + \Delta t} \boldsymbol{\sigma}_{\text{tr}} + \frac{\Delta t}{\beta + \Delta t} \bar{\boldsymbol{\sigma}},$$

being a convex combination of the elastic ($\beta = \infty$) and perfect elasto-plastic response ($\beta = 0$). Though time has a physical meaning in viscoplasticity, the material response only depends on the quotient $\frac{\Delta t}{\beta}$ and therefore the considered time horizon $[0, 3.5]$ with $\Delta t = 0.1$ is artificial.

The material parameters can be found in Table 5.

Material parameters			
Shear modulus:	μ	5.5	MPa
Bulk modulus:	κ	12.07	MPa
Cohesion:	c	0.008	MPa
Friction angle:	ϕ	25°	
Dilatancy angle:	ψ	5°	
Scaling factor:	k_0	0.7	
Specific weight:	γ	0.033	MPa/m
Viscoplasticity:	β	0.0005	s

Computational details			
Degrees of freedom	3	826 995	
on mesh refinement	4	6 452 451	
level (MRL)	5	50 973 123	
Final time:	T	3.5	s
Time step size:	Δt	0.1	s

Table 5: Parameters for the slope failure problem.

Within Ω , a body force is prescribed (gravity) and on a part of the upper boundary (the blue shaded area in Figure 2), a traction force applies. The loading regime is as follows: up to time $\hat{t} = 1$, the gravity force is applied incrementally and afterwards kept constant, whereas no traction force is applied up to \hat{t} . Beyond \hat{t} , the traction force is increased linearly with time.

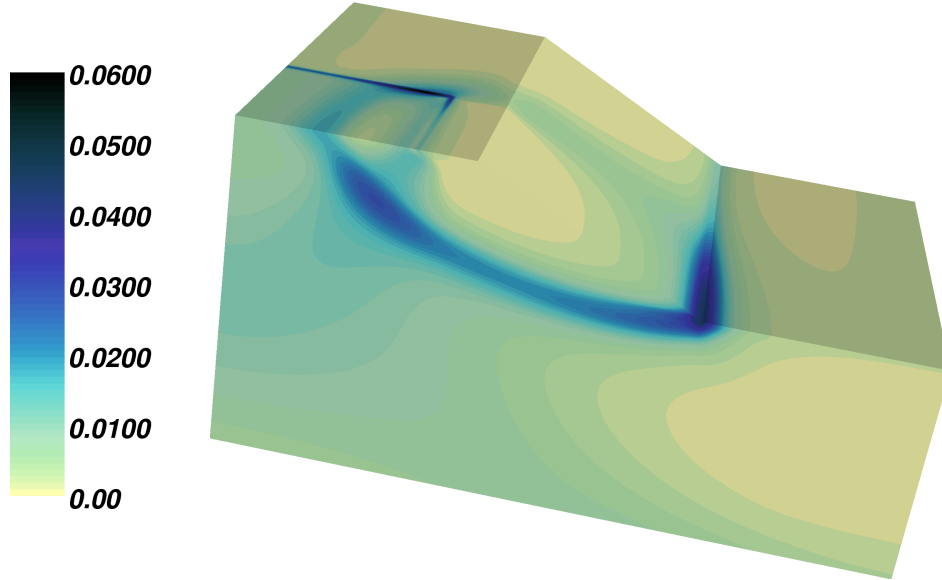


Figure 3: Accumulated plastic strain at time $t = 2.9$

As a result of the geometry, during the gravity loading phase, the deformation is homogeneous w.r.t. the x_1 -direction. After $t = \widehat{t}$, the deformation is fully 3d since the traction force triggers a shear band. With the functions $L_g = \min\{t, \widehat{t}\}$ and $L_t(t) = \max\{0, t - \widehat{t}\}$, $\mathbf{b} = [0, 0, -\gamma]^T$, $\mathbf{t}_N = [0, 0, -1/400]^T$ and the surface $\Gamma_N = (0, 3) \times (9, 12) \times \{6\}$, the load functional (2.14) takes the form

$$\ell(t, \mathbf{w}) = L_g(t) \int_{\Omega} \mathbf{b} \cdot \mathbf{w} \, dx + L_t(t) \int_{\Gamma_N} \mathbf{t}_N \cdot \mathbf{w} \, da.$$

The loading process is also illustrated in Figure 2(b). The slope geometry is such that plastic behavior already sets on in the gravity loading phase, i.e. the self-weight of the slope triggers plastic deformation.

k	Mesh refinement level		
	MRL 3	MRL 4	MRL 5
0	2.7e-04	1.9e-04	1.1e-04
1	5.7e-05	5.3e-05	6.2e-05
2	3.7e-06	1.5e-05	3.4e-05
3	4.9e-07	1.7e-06	6.9e-06
4	4.8e-10	2.2e-07	5.3e-07
5		7.8e-09	1.1e-07
6		6.1e-12	2.6e-08
7			3.1e-09
8			5.5e-11

Table 6: Slope failure problem: convergence of the (outer) generalized Newton iteration for Drucker-Prager plasticity at time step 29 for different mesh refinement levels (MRL), also see Table 5.

Table 6 shows the convergence on different levels of mesh refinement. We observe fast superlinear convergence for all levels of mesh refinement, but the number of iterations is mesh-dependent. This generally seems to hold true for problems in

elasto-plasticity, since it was not possible so far, to prove super-linear convergence in a function space setting, cf. Gruber and Valdman (2009) for more details. Finally, Figure 3 gives an illustration of the accumulated plastic strain $\int_0^t |\dot{\boldsymbol{\epsilon}}_p(s)| \, ds$ at time $t = 2.9$ and we observe the formation of a shear band.

Appendix A. Semismooth Newton methods

For convenience of the reader we collect the results on semismooth functions which are used in Sect. 3-8, see also Pang and Facchinei (2003a,b). Here, we restrict ourselves to the Euclidean case. For a corresponding calculus in function spaces, see, e.g., Chen et al. (2000); Hintermüller et al. (2003); Ito and Kunisch (2008).

A.1. Generalized derivatives

Let $F: \mathbb{R}^N \rightarrow \mathbb{R}^M$ be a continuous function. Then, F is directional differentiable at x in direction $h \in \mathbb{R}^N$, if the limit

$$DF(x; h) := \lim_{t \downarrow 0} \frac{1}{t} (F(x + th) - F(x))$$

exist, and F is B(ouligand)-differentiable if additionally

$$\frac{1}{|h|} (F(x + h) - F(x) - DF(x; h)) = o(|h|) \quad \text{as } h \rightarrow 0, h \neq 0.$$

In the following, we always assume that F is Lipschitz continuous. Then, F is B-differentiable if and only if F is directionally differentiable. Moreover, by Rademacher's theorem (Clarke et al., 1998), the set of points $\Theta_F \subset \mathbb{R}^N$ where F is differentiable is dense. For $x \in \mathbb{R}^N$, we define the B(ouligand)-subdifferential by

$$\partial^B F(x) = \{B \in \mathbb{R}^{M,N} : B = \lim_{y \rightarrow x, y \in \Theta_F} DF(y)\}, \quad (\text{A.1})$$

and Clarke's generalized Jacobian is its convex hull

$$\partial F(x) = \text{conv} \{ \partial^B F(x) \} \supset \partial^B F(x). \quad (\text{A.2})$$

Note that $\partial^B F(x) = \partial F(x) = \{DF(x)\}$ for $x \in \Theta_F$.

The function F is called CD-regular at x , if all matrices in $\partial F(x)$ are regular.

Proposition A.1. (Pang and Facchinei, 2003b, Thm. 7.5.3) *If F is CD-regular at x^* , $\delta > 0$ exists such that F is CD-regular at all $x \in \{y \in \mathbb{R}^N : |x^* - y| < \delta\}$.*

A.2. Semismooth functions

The function F is *semismooth* at x , if it is locally Lipschitz continuous at x and if the limit

$$\lim_{\substack{V \in \partial F(x+th'), \\ t \downarrow 0, h' \rightarrow h}} Vh' \quad (\text{A.3})$$

exists for all $h \in \mathbb{R}^N$.

Proposition A.2. (Qi and Sun, 1993; von Heusinger and Kanzow, 2008). *For F , the following statements are equivalent:*

1. F is semismooth at x .
2. F is locally Lipschitz at x , $DF(x; \cdot)$ exists and for any $G \in \partial F(x+h)$:

$$|Gh - DF(x; h)| = o(|h|) \quad \text{as } h \rightarrow 0.$$

3. F is locally Lipschitz at x , $DF(x; \cdot)$ exists and for any $G \in \partial F(x+h)$:

$$|F(x+h) - F(x) - Gh| = o(|h|) \quad \text{as } h \rightarrow 0.$$

4. For all $G \in \partial^B F(x+h)$: $|Gh - DF(x; h)| = o(|h|)$ as $h \rightarrow 0$.
5. F_i is semismooth for all components $i = 1, \dots, M$, i.e. for all $H_i \in \partial F_i(x+h)$ we have $|H_i h - DF_i(x; h)| = o(|h|)$ as $h \rightarrow 0$.

If $o(|h|)$ can be replaced by $O(|h|^{1+s})$, $s \in (0, 1]$, we call F semismooth of order s , and in case $s = 1$, we say F is *strongly semismooth*.

For semismooth functions, the following chain rule holds.

Proposition A.3. (Pang and Facchinei, 2003b, Prop. 7.4.4). *Let $F: \mathbb{R}^N \rightarrow \mathbb{R}^M$ be (strongly) semismooth in a neighborhood of $\hat{x} \in \mathbb{R}^N$ and let $G: \mathbb{R}^M \rightarrow \mathbb{R}^P$ be (strongly) semismooth in a neighborhood of $F(\hat{x})$. Then $H: \mathbb{R}^N \rightarrow \mathbb{R}^P$, $H = G \circ F$ is (strongly) semismooth in a neighborhood of \hat{x} .*

For $T: \mathbb{R}^N \times \mathbb{R}^M \rightarrow \mathbb{R}^N$ we define

$$\partial_x T(x, y) = \{A_x \in \mathbb{R}^{N,N} : A_y \text{ exists s.t. } [A_x A_y] \in \partial T(x, y)\}.$$

In the same way we define $\partial_y T(x, y) \subset \mathbb{R}^{N,M}$.

Proposition A.4. (Gowda, 2004; von Heusinger and Kanzow, 2008) *Let T be semismooth in a neighborhood of a point (x^*, y^*) satisfying $T(x^*, y^*) = 0$, and let all matrices $\partial_x T(x^*, y^*)$ be nonsingular. Then, there exists an open neighborhood $U(y^*)$ of y^* and a function $Y: U(y^*) \rightarrow \mathbb{R}^N$ which is locally Lipschitz and semismooth such that $Y(y^*) = x^*$ and $T(Y(y), y) = 0$ for all $y \in U(y^*)$. Moreover, if $[A_x A_y] \in \partial^B T(Y(y), y)$, we have*

$$-A_x^{-1} A_y \in \partial^B Y(y) \subset \partial Y(y).$$

A.3. A generalized Newton method

A generalized Newton iteration to compute a root x^* of a Lipschitz continuous function $F: \mathbb{R}^N \rightarrow \mathbb{R}^N$ is defined by

$$x^k = x^{k-1} - G_k^{-1} F(x^{k-1}), \quad G_k \in \partial F(x^{k-1}), \quad k \geq 1. \quad (\text{A.4})$$

Proposition A.5. (Qi and Sun, 1993). *Let x^* be a solution of $F(x^*) = 0$. Assume that F is semismooth (of order s) and CD-regular at x^* . Then, provided that $|x^0 - x^*|$ is small enough, the iteration (A.4) is well-defined and converges superlinearly (with order $1 + s$) to the solution x^* .*

The *proof* is based on Proposition A.1 showing that the iteration is well-defined and the superlinear convergence (with order $1 + s$) then follows from property 3. in Proposition A.2.

A.4. Semismoothness of projection operators

Let $A \in \mathbb{R}^{N,N}$ be symmetric positive definite, let $(x, y)_A = x^T A y$ be an inner product in \mathbb{R}^N with norm $|x|_A = \sqrt{(x, x)_A}$, and let $K \subset \mathbb{R}^N$ be a convex set. Then, the orthogonal projection $P: \mathbb{R}^N \rightarrow K \subset \mathbb{R}^N$ is well defined and uniquely characterized by

$$(x - P(x), z - P(x))_A \leq 0 \quad z \in K.$$

Note that P is non-expansive, i.e., $|P(x) - P(y)|_A \leq |x - y|_A$.

In the case when $K = \{x \in \mathbb{R}^N : f_i(x) \leq 0, i = 1, \dots, p\}$ with convex functions $f_i: \mathbb{R}^N \rightarrow \mathbb{R}$, the projection $x^* = P(y)$ and the corresponding Lagrange multiplier $\lambda \in \mathbb{R}^p$, $\lambda \geq 0$ are characterized as a saddle point of the Lagrangian

$$L(x, \lambda) = \frac{1}{2} |x - y|_A^2 + \lambda^T f(x).$$

Proposition A.6. *Let $f \in C^2(\mathbb{R}^N, \mathbb{R}^p)$ be convex and let $x := P(y) \in K$ be the projection of y onto K . Furthermore assume that the constant rank constraint qualification (CRCQ) holds at x , i.e., there is a neighborhood U of x such that for each subset $J \subset I(x)$ of the active indices $I(x) := \{i \in \{1, \dots, p\} : f_i(x) = 0\}$ and all $z \in U$, the matrices $Df(z)_{j \in J}$ have the same rank. Then, the projection P is semismooth at y .*

A *proof* can be found in (Sauter, 2010, Theorem A.11) and is based on results given in Pang and Ralph (1996); Pang and Facchinei (2003a,b). We remark that also a characterization of the directional derivative $DP(y; h)$ exists which is a projection in a distorted metric onto the critical cone (Pang and Ralph, 1996). For $y \in K$, this coincides with the projection onto the tangent cone, cf. Zarantonello (1971). We remark that the (CRCQ) is implied by the *linear independence constraint qualification* (LICQ) but not by (and neither implies) the *Mangasarian-Fromowitz constraint qualification* (MFCQ).

In some special cases no constraint qualification is necessary.

Proposition A.7. *If K is a polyhedron or the second order unit cone, i.e., $B \in \mathbb{R}^{p,N}$ and $d \in \mathbb{R}^p$ exist such that*

$$K = \{x \in \mathbb{R}^N : Bx \leq d\} \quad \text{or} \\ K = \{x \equiv (\hat{x}, x_0) \in \mathbb{R}^{N-1} \times \mathbb{R} : |\hat{x}| \leq x_0\},$$

the orthogonal projection onto K is strongly semismooth.

The result follows from (Pang and Facchinei, 2003b, Prop. 7.4.7) in the polyhedral case, and from Hayashi et al. (2005); Goh and Meng (2006) for the second order unit cone.

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