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Averaging techniques for reliable a posteriori FE-error control in elastoplasticity with hardening

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Abstract

Averaging techniques are popular tools in adaptive finite element methods for numerical simulation in continuum mechanics since they provide efficient a posteriori error control. In this paper, the reliability of *any* averaging estimator is shown for low order finite element methods in one time-step of elastoplasticity with hardening. The constants and higher-order terms are effected by the hardening and the smoothness of given right-hand sides, but are independent of the structure of a shape-regular mesh. Since it involves a different functional analytical framework, the case of perfect plasticity is excluded from this paper.

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1. Introduction

Within a spatial discretisation of one time-step in a finite element analysis of elastoplasticity, we encounter a variational inequality with a quite complicated material law determined by admissible (generalised) stresses on top of the problem of linear elasticity.

It is therefore not at all clear that a simple averaging of the discrete stress field might serve as an error estimator for reliable error control. In particular, the residual in the material law, e.g., in some Kuhn–Tucker conditions on the plastic multiplier, might have to be involved. This paper shows that indeed, *any* stress-averaging technique [32] is reliable.

The main results concern a piecewise stress approximation σ_h (to the exact stress σ) obtained by a standard finite element analysis of one time-step within the evolution of an elastoplastic (or viscoplastic)

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body Ω with piecewise constant hardening approximations and globally continuous piecewise linear displacement approximants [14,27].

A posteriori error estimates employ the information available after the computation of σ_h and determine computable error estimators η as error bounds: The error estimator η is called *reliable* if the stress error e in energy norm,

$$e^2 := \|\mathbb{C}^{-1/2}(\sigma - \sigma_h)\|_{L^2(\Omega)}^2 := \int_{\Omega} (\sigma - \sigma_h) : \mathbb{C}^{-1}(\sigma - \sigma_h) \, d\Omega, \quad (1.1)$$

(where \mathbb{C} is the constant fourth-order elasticity tensor), is bounded from above by η ,

$$e \leq C_1 \eta. \quad (1.2)$$

Strictly speaking, an estimator is efficient if the converse estimate holds. In a relaxed form, we consider an error estimator η as efficient if (h.o.t. replaces terms of higher order)

$$\eta \leq C_2 e + \text{h.o.t.} \quad (1.3)$$

The estimates (1.2) and (1.3) involve constants C_j which are independent of the number N of degrees of freedom or the mesh-size and also independent of the unknown exact solution; they may depend on the domain, the material law and parameters, and on applied volume and surface loads f and g , respectively. The higher order terms in (1.3) may depend on the exact solution.

The first reliable error estimators were established in [18] even for perfect plasticity and involve terms such as

$$\eta_{T,R} = h_T^2 \int_T |f + \text{div}_{\mathcal{T}} \sigma_h|^2 \, d\Omega + \int_{\partial T} h_E |[\sigma_h \cdot n_E]|^2 \, ds \quad (1.4)$$

for one element T (of diameter h_T) with edges E (of length h_E) on the boundary ∂T ; f is a given volume force and $\text{div}_{\mathcal{T}} \sigma_h$ is the piecewise divergence (which vanishes in the present case of lowest order fem) while $[\sigma_h \cdot n_E]$ denotes the jump of the stress vectors across the element edge E with normal n_E (and standard modification on parts of the boundary of Ω with applied surface loads).

The residual-based estimator [18] involves other terms in the plastic region where the functional analytical setting required for perfect plasticity provides only very weak approximation properties of the displacement field in $\text{BD}(\Omega)$ [15,25–29]. The resulting estimate (1.2) of [18] therefore involves a moderate constant C_1 but is (probably) *not* efficient. Numerical experiments show a high mesh-refinement in the plastic part of the body which appear unreasonable from the approximation property of the exact solution (but certainly is unavoidable from the rigorous mathematical viewpoint).

The duality approach in [22–24] allows for more general error norms (or error functionals) and cures the difficulty with a possibly non-smooth solution with a recovery of (unknown) higher derivatives of the exact solution in computable differences of its finite element approximation. This indicates roughness of the unknown solution, adopts the mesh-refinement to it, and performs remarkably well in their numerical examples. The rigorousness of their estimate, however, is disputable; but it seems fair to say that their approach leads to very accurate error guesses and is very valuable for particular error functionals.

This paper is restricted to the error norms e of (1.1) and continuous our mathematical analysis in [3,6–8] with focus on elastoplasticity with hardening, where the functional analytical context of linear elasticity is applicable on the price of that some constants may crucially depend on the hardening moduli. As shown in [3,8], (1.4) yields indeed a reliable and efficient error estimator

$$\eta_R = \left(\sum_{T \in \mathcal{T}} \eta_T^2 \right)^{1/2}. \quad (1.5)$$

At first glance it may surprise that this error estimator is the same as in the context of linear elasticity (of course with a different dependence of the stress from the strain and hardening variables). The reason is that the evolution problems in the plastic material law is (within one time-increment) are satisfied *exactly* on each element whence the material law has a vanishing residual. Thus, excluding the error accumulation for progressing time-steps, the only remaining residuals are the discrete equilibrium conditions of (1.4).

This paper addresses the question of reliable and efficient estimators which are based on averaging techniques for unstructured grids in the presence of hardening. The accumulating error of the time-discretisation attracted experimentalists to estimate the error with averaging techniques [20,21]. In Hencky elastoplasticity under question, this accounts for a substitution of the (unknown) exact stress σ in (1.2) by *some* computed average σ_h^* ,

$$\eta_Z := \left(\sum_{T \in \mathcal{T}} \eta_{T,Z}^2 \right)^{1/2} \tag{1.6}$$

with the elementwise contributions

$$\eta_{T,Z}^2 := \|\mathbb{C}^{-1/2}(\sigma_h^* - \sigma_h)\|_{L^2(T)}^2 := \int_T (\sigma_h^* - \sigma_h) : \mathbb{C}^{-1}(\sigma_h^* - \sigma_h) \, d\Omega. \tag{1.7}$$

Note that (1.7) and so η_Z involves the stresses (without hardening parameters) while [20] treats generalised stress fields (where the hardening parameters are averaged as well). Without a mathematical justification, it is not at all clear which variables should enter the averaging process: Besides the discrete stress variables there are other internal variables, the discrete strain field (whose curvature is certainly important for mesh-refinements), and possibly approximations to plastic multipliers.

The classical justification of averaging techniques advertised by Zienkiewicz and Zhu is based on superconvergence phenomena which are available for structured grids and smooth solutions only and have not been verified in elastoplasticity at all.

Following our technique for the justification of the ZZ-estimator in [4,10,11] based on a special approximation operator [5,12], we prove in this paper the reliability and efficiency of η_Z for an arbitrary globally continuous and piecewise polynomial approximation σ_h^* which is supposed to satisfy static boundary conditions at nodal points \mathcal{N} there. To state the main results for a piecewise smooth applied surface load g on Γ_N with edges \mathcal{E}_N , let

$$\mathcal{Q}(\mathcal{T}, g) := \{ \sigma_h^* \in \mathcal{S}^1(\mathcal{T})^{d \times d} : \sigma_h^*(z) \cdot n_E = g(z) \text{ for all } z \in \mathcal{N} \cap E \text{ with } E \in \mathcal{E}_N \}. \tag{1.8}$$

Then, *any* average $\sigma_h^* \in \mathcal{Q}(\mathcal{T}, g)$ leads in (1.7) to a reliable estimate. In particular the minimal choice

$$\eta_Z^{(\text{opt})} := \min_{\sigma_h^* \in \mathcal{Q}(\mathcal{T}, g)} \|\mathbb{C}^{-1/2}(\sigma_h^* - \sigma_h)\|_{L^2(\Omega)} \tag{1.9}$$

is reliable but costly to compute. However, $\eta = \eta_Z^{(\text{opt})}$ yields a reliable and efficient estimate with $C_2 = 1$, i.e., we have

$$e - \text{h.o.t.} \leq C_1 \eta_Z^{(\text{opt})} \leq C_1 e + \text{h.o.t.} \tag{1.10}$$

Note that the second inequality of (1.10) follows from a triangle inequality for a nodal interpolant $I\sigma \in \mathcal{Q}(\mathcal{T}, g)$ of σ ; indeed,

$$\eta_Z^{(\text{opt})} \leq \|\mathbb{C}^{-1/2}(\sigma_h - I\sigma)\|_{L^2(\Omega)} \leq \|\mathbb{C}^{-1/2}(\sigma - I\sigma)\|_{L^2(\Omega)} + \|\mathbb{C}^{-1/2}(\sigma - \sigma_h)\|_{L^2(\Omega)} = e + \text{h.o.t.},$$

as then $\|\mathbb{C}^{-1/2}(\sigma - I\sigma)\|_{L^2(\Omega)}$ is of higher order. It is worth mentioning that, even for perfect plasticity, the exact stress σ is smooth (in contrast to the displacement field) [25,26]; hence there holds efficiency with a constant 1.

This paper concerns the remaining crucial reliability estimate of (1.10), studies the dependencies of the constants C_j and the higher-order terms h.o.t., and proposes a related adaptive algorithm for efficient automatic mesh-refining.

The rest of this paper is organised as follows. Hencky plasticity reads as a variational inequality and so we address the problem accordingly from an abstract point of view in Section 2. It turns out that this abstract frame covers a large class of material laws in the dual (i.e., stress-oriented) and primal (i.e., strain-oriented) formulation. Both models are introduced and analysed in Section 3 for an abstract material law. Von Mises yield functions with isotropic and/or kinematic hardening or viscoplasticity are covered as particular cases in Section 4. The numerical examples of Section 5 are striking in the sense that a comparison with an exact solution shows that our realisation of the ZZ-estimator (1.6) is amazingly close to the exact stress error e . The proposed adaptive Algorithm 1 improved the spatial discretisation significantly.

Throughout the paper, we employ standard notation for Lebesgue and Sobolev spaces, and $(\cdot; \cdot)$ denotes the inner product of (any power of) $L^2(\Omega)$.

2. Abstract frame

One time-step of an elastoplastic evolution problem with hardening or viscoplastic regularisation yields the following task: Find a solution x in a convex, closed set \mathcal{K} to the variational inequality

$$\ell(y - x) \leq a(x; y - x) + \psi(y) - \psi(x) \quad \text{for all } y \in \mathcal{K}. \quad (2.1)$$

With a Hilbert space X , $a : X \times X \rightarrow \mathbb{R}$ is a continuous symmetric bilinear form, $\ell : X \rightarrow \mathbb{R}$ a continuous and linear functional and $\psi : X \rightarrow [0, \infty]$ is a convex, lower semicontinuous mapping which is not identically equal to ∞ . Ellipticity of a is sufficient for the existence of a solution which minimises the energy functional $\frac{1}{2}a(x, x) - \ell(x) + \psi(x)$ on \mathcal{K} [31].

A finite element discretisation of X yields a discrete set $\mathcal{K}_h \subseteq \mathcal{K} \subseteq X$; since $\mathcal{K}_h \subseteq \mathcal{K}$ the discretisation is conforming. Suppose that $\bar{x} \in \mathcal{K}_h$ exists with $\psi(\bar{x}) \leq \psi(x)$.

Similar ellipticity conditions on a and on the convexity and closedness of \mathcal{K}_h (as in the aforementioned continuous case) show the existence of a solution $x_h \in \mathcal{K}_h$ to the discrete variational inequality

$$\ell(y_h - x_h) \leq a(x_h; y_h - x_h) + \psi(y_h) - \psi(x_h) \quad \text{for all } y_h \in \mathcal{K}_h. \quad (2.2)$$

In the next theorem, ellipticity of a is not explicitly required.

Theorem 1. *Suppose $x \in \mathcal{K}$ solves (2.1) and $x_h \in \mathcal{K}_h$ solves (2.2). Then we have*

$$a(x - x_h; x - x_h) \leq \min_{y_h \in \mathcal{K}_h} (a(x_h; y_h - x) - \ell(y_h - x) + \psi(y_h) - \psi(x)). \quad (2.3)$$

Proof. Set $y = x_h \in \mathcal{K}_h \subseteq \mathcal{K}$ in (2.1) and set $y_h \in \mathcal{K}_h$ in (2.2). Adding the resulting inequalities we infer $\ell(y_h - x) \leq a(x; x_h - x) + a(x_h; y_h - x_h) + \psi(y_h) - \psi(x)$ from which we deduce (2.3) even for a non-symmetric non-elliptic bilinear form a . \square

The theorem will be evaluated for some $y_h \in \mathcal{K}_h$ which simultaneously satisfies $y_h \approx x$ and $\psi(y_h) \leq \psi(x)$. The point is that without the latter property we have no argument to see that $|\psi(y_h) - \psi(x)|$ is small since ψ is not smooth. The essential idea of [8] is to use Jensen's inequality and choose parts of y_h as the (elementwise) integral means of x .

Theorem 2 (Jensen's inequality for integrals). *Suppose $j : \mathbb{R}^m \rightarrow [0, \infty)$ is convex, $\omega \subseteq \mathbb{R}^d$ is an open and bounded set with d -dimensional measure $|\omega|$. For $p \in L^1(\omega)^m$ with mean $\bar{p} := \int_{\omega} p \, d\Omega / |\omega| \in \mathbb{R}^m$ we have*

$$\int_{\omega} j(\bar{p}) \, d\Omega \leq \int_{\omega} j(p) \, d\Omega. \tag{2.4}$$

Proof. The proof is to stress the difference to the point-version

$$j\left(\sum_{k=1}^N \lambda_k p_k\right) \leq \sum_{k=1}^N \lambda_k j(p_k) \tag{2.5}$$

for $0 \leq \lambda_1, \dots, \lambda_N \leq 1$ with $\lambda_1 + \dots + \lambda_N = 1$ and $p_1, \dots, p_N \in \mathbb{R}^m$. The estimate (2.5) is occasionally called Jensen inequality: it is directly related to the convexity of j . Indeed, if p is a simple function, i.e., $p = \sum_{k=1}^N p_k \chi_{A_k}$ for $p_1, \dots, p_N \in \mathbb{R}^m$ and a partition $A_1 \cup \dots \cup A_N = \omega$ of ω , with characteristic functions $\chi_{A_k}(x) = 1$ if $x \in A_k$ and $= 0$ otherwise, we have convex coefficients $\lambda_k := |A_k|/|\omega|$ and deduce from (2.5) that (2.4) holds. It remains to verify (2.4) for an arbitrary function p in $L^1(\omega)^m$ by density of simple functions. The limit process in $L^1(\omega)$ is technical and hence omitted; we refer to [19] for a proof. \square

3. Reliability of stress-averaging techniques in elastoplasticity

This section is devoted to the primal and dual formulation of elastoplasticity and to put the abstract frame in a precise setting. We start with the dual formulation (in the notation of [14]) which is stress-related and more frequently found in the engineering literature. The equilibrium conditions read

$$\operatorname{div} \sigma + f = 0 \quad \text{in } \Omega, \tag{3.1}$$

$$\sigma n = g \quad \text{on } \Gamma_N \tag{3.2}$$

for the stress tensor $\sigma \in L^2(\Omega; \mathbb{R}_{\text{sym}}^{d \times d})$ in a body Ω , a bounded Lipschitz domain in \mathbb{R}^d with boundary $\Gamma = \Gamma_D \cup \Gamma_N$. On some closed part Γ_D of Γ with positive surface measure we suppose homogeneous geometric boundary conditions for the displacement field u ,

$$u \in H := H_D^1(\Omega) := \{v \in H^1(\Omega)^d : v = 0 \text{ on } \Gamma_D\}.$$

On the remaining part $\Gamma_N := \Gamma \setminus \Gamma_D$, the traction is prescribed by a given $g \in L^2(\Gamma_N)^d$ and the outer unit normal n . With the fourth-order elasticity tensor \mathbb{C} , $\mathbb{C}\tau = 2\mu\tau + \operatorname{tr} \tau \operatorname{Id}$, we suppose an additive split $\varepsilon(u) = \mathbb{C}^{-1}\sigma + p$ of the (linear) Green strain

$$\varepsilon(u) = \operatorname{sym} Du = ((u_{j,k} + u_{k,j})/2 : j, k = 1, \dots, d).$$

With further internal (hardening) variables $\alpha \in L^2(\Omega)^m$ and the hardening tensor $\mathbb{H} \in \mathbb{R}_{\text{sym}}^{m \times m}$ we suppose a material law

$$(\varepsilon(u) - \mathbb{C}^{-1}\sigma) : (\tau - \sigma) + \alpha \cdot \mathbb{H}^{-1}(\beta - \alpha) \leq j(\tau, \beta) - j(\sigma, \alpha) \tag{3.3}$$

for all $(\tau, \beta) \in \mathbb{R}_{\text{sym}}^{d \times d} \times \mathbb{R}^m$. The plastic potential $j : \mathbb{R}_{\text{sym}}^{d \times d} \times \mathbb{R}^m \rightarrow [0, \infty]$ takes the value $+\infty$ for generalised stresses (σ, α) which are not admissible. Examples will be listed at the end of this section and indeed, it will be shown that our results are quite independent of the choice of j . It is merely supposed that j is convex, lower semi-continuous, and proper (i.e., not $j \equiv +\infty$) and that hardening parameters guarantee definiteness of the bilinear form.

The problem in the dual formulation (D) reads for one time-step: Seek $(u, \sigma, \alpha) \in H \times L$, $L := L^2(\Omega; \mathbb{R}_{\text{sym}}^{d \times d} \times \mathbb{R}^m)$ satisfying (3.1)–(3.3). We refer to [15–17, 25, 26, 28, 29] for details on existence, uniqueness, and regularity of solutions to (D).

The discrete problem (D_h) involves a regular triangulation \mathcal{T} (in triangles if $d = 2$ or tetrahedrons if $d = 3$ etc.) of the domain Ω (no hanging nodes, $\cup \mathcal{T}$ matches $\bar{\Omega}$ exactly). Let $\mathcal{L}^k(\mathcal{T})$ denote the (in general discontinuous) \mathcal{T} -piecewise polynomials of degree $\leq k$ and set

$$H_h := \mathcal{S}_D^1(\mathcal{T}) := \{v_h \in H_D^1(\Omega) : v_h \in \mathcal{L}^1(\mathcal{T})^d\},$$

$$L_h := \mathcal{L}^0(\mathcal{T}; \mathbb{R}_{\text{sym}}^{d \times d} \times \mathbb{R}^m) := \{(\tau, \beta) \in L : \forall T \in \mathcal{T}, (\tau, \beta)|_T \in \mathbb{R}_{\text{sym}}^{d \times d} \times \mathbb{R}^m\}.$$

Discrete problem (D_h) : Seek $(u_h, \sigma_h, \alpha_h) \in H_h \times L_h$ satisfying, for all $(v_h, \tau_h, \beta_h) \in H_h \times L_h$,

$$(\sigma_h; \varepsilon(v_h)) = (f; v_h) + \int_{\Gamma_D} g \cdot v_h \, ds, \tag{3.4}$$

$$(\varepsilon(u_h) - \mathbb{C}^{-1}\sigma_h; \tau_h - \sigma_h) + (\alpha_h; \mathbb{H}^{-1}(\alpha_h - \beta_h)) \leq \int_{\Omega} j(\tau_h, \beta_h) \, d\Omega - \int_{\Omega} j(\sigma_h, \alpha_h) \, d\Omega. \tag{3.5}$$

We refer to [7,15,16] for details, e.g., on existence and uniqueness of discrete solutions and mention only that (3.4) is the discrete weak form of (3.1), (3.2) and (3.5) is the discrete (equivalent) integral form of (3.3).

Theorem 3. The problem (D) (resp. (D_h)) is equivalent to (2.1) (resp. (2.2)) provided $\mathcal{X} = X = H \times L$ (resp. $\mathcal{X}_h = H_h \times L_h \subseteq \mathcal{X}$) and, for $x = (u, \sigma, \alpha), y = (v, \tau, \beta) \in X$,

$$a(x, y) = (\sigma; \mathbb{C}^{-1}\tau) + (\alpha; \mathbb{H}^{-1}\beta) - (\sigma; \varepsilon(v)),$$

$$\ell(y) = -(f; v) - \int_{\Gamma_N} g \cdot v \, ds,$$

$$\psi(y) = \int_{\Omega} j(\tau, \beta) \, d\Omega.$$

Proof. Standard arguments (such as integration by parts) verify the assertion. \square

A consequence of Theorems 1 and 2 is that the nonlinear problem (D) resp. (D_h) can be treated as the linear case of [11]; $\partial_{\varepsilon} g / \partial s$ is the \mathcal{E} -piecewise derivative along Γ_N .

Theorem 4. Let (u, σ, α) solve (D) and $(u_h, \sigma_h, \alpha_h)$ solve (D_h) . Then

$$\|(u - u_h, \sigma - \sigma_h, \alpha - \alpha_h)\|_{H \times L} \leq c_1(\eta_Z + \|[h_{\mathcal{E}}^{3/2} \partial_{\varepsilon} g / \partial s]\|_{L^2(\Gamma_N)} + \|h_{\mathcal{T}} \nabla f\|_{L^2(\Omega)}). \tag{3.6}$$

The constant $c_1 > 0$ depends on the shape of the elements (minimum angle condition), on the material parameters and on the type of hardening or viscoplastic regularisation.

Proof. With the definitions of Theorem 3, Theorem 1 and the ellipticity of \mathbb{C} and \mathbb{H} yield

$$c_2 \|(\sigma - \sigma_h, \alpha - \alpha_h)\|_L^2 \leq a(x - x_h; x - x_h) \leq a(x_h; y_h - x) - \ell(y_h - x) + \psi(y_h) - \psi(x) \tag{3.7}$$

for all $y_h = (v, \tau_h, \beta_h) \in \mathcal{X}_h$. Given (σ, α) , let (τ_h, β_h) be its \mathcal{T} -piecewise integral mean,

$$(\tau_h, \beta_h)|_T := \int_T (\sigma, \alpha) \, d\Omega / |T| \in \mathbb{R}_{\text{sym}}^{d \times d} \times \mathbb{R}^m \quad \text{for all } T \in \mathcal{T}$$

and employ Theorem 2 for $\omega := T$ and $p := (\sigma, \alpha)|_T$. A summation of the resulting inequality (2.4) over all $T \in \mathcal{T}$ shows

$$\psi(y_h) - \psi(x) = \int_{\Omega} j(\tau_h, \beta_h) \, d\Omega - \int_{\Omega} j(\sigma, \alpha) \, d\Omega \leq 0. \tag{3.8}$$

In the remaining terms of $a(x_h, y_h - x)$ the difference $\sigma - \tau_h$ (and similarly $\alpha - \beta_h$) has integral mean zero over each element. Hence, e.g., the product $(\sigma_h; \mathbb{C}^{-1}(\sigma - \tau_h)) = 0$ as \mathbb{C} is constant in space and $\sigma_h|_T$ is constant on each $T \in \mathcal{T}$. These arguments show in (3.7) and (3.8)

$$\begin{aligned} c_2 \|(\sigma - \sigma_h, \alpha - \alpha_h)\|_L^2 &\leq (f; v_h - u) + \int_{\Gamma_N} g \cdot (v_h - u) \, ds - (\sigma_h; \varepsilon(v_h - u)) \\ &= (\sigma_h; \varepsilon(e - e_h)) - (f; e - e_h) - \int_{\Gamma_N} g \cdot (e - e_h) \, ds = -(\sigma - \sigma_h; \varepsilon(e - e_h)) \end{aligned} \tag{3.9}$$

for $e := u - u_h$ and $v_h := u_h + e_h$ with arbitrary $e_h \in \mathcal{S}_D^1(\mathcal{T})$. The Section 5 in [11] studies exclusively the linear case $(\sigma - \sigma_h; \varepsilon(e - e_h))$ and proves with a certain choice of $e_h = Je$ from [4,5,12] that

$$|(\sigma - \sigma_h; \varepsilon(e - e_h))| \leq c_3 \|e\|_{H^1(\Omega)} (\eta_Z + \| [h_\varepsilon^{3/2} \partial_\varepsilon g / \partial s] \|_{L^2(\Gamma_N)} + \| h_{\mathcal{F}} \nabla f \|_{L^2(\Omega)}). \tag{3.10}$$

For the proof, we refer to [11] and mention only that c_3 depends on the shape of the elements and patches. The final argument essentially utilises the hardening to derive the estimate

$$\|\varepsilon(e)\|_{L^2(\Omega)} \leq c_4 \|(\sigma - \sigma_h, \alpha - \alpha_h)\|_L \tag{3.11}$$

with a hardening-depending constant $c_4 > 0$ as in [7, Lemma 5.4], [8, Theorem 4.2], [3, Remark 5.5], or in earlier work [16,17] of Johnson for isotropic or kinematic hardening or viscoplastic regularisation. Combining (3.9)–(3.11) with Korn’s inequality, $\|e\|_{H^1(\Omega)} \leq c_5 \|\varepsilon(e)\|_{L^2(\Omega)}$, we conclude the proof of (3.6). \square

The primal formulation of elastoplasticity is equivalently obtained from (D) by the duality principle in convex analysis: $x \in \partial j(y)$ is equivalent to $y \in \partial j^*(x)$ which leads to

$$\sigma : (q - p) + a \cdot (b - a) \leq j^*(q, b) - j^*(p, a). \tag{3.12}$$

Here $p := \varepsilon(u) - \mathbb{C}^{-1}\sigma$, $a := -\mathbb{H}^{-1}\alpha$, and j^* is the dual, also called Fenchel transform or conjugate functional,

$$j^*(x) = \sup_{y \in \mathbb{R}^{d \times d}_{\text{sym}} \times \mathbb{R}^m} (x * y - j(y)).$$

For the proof of the equivalence of (3.3) and (3.12) we refer to textbooks about convex analysis [13,31] and the literature on the primal formulation [2,5,14]. The primal formulation (P) reads: Seek $(u, p, a) \in H \times L$ satisfying (3.1), (3.2) and (3.12) for $\sigma := \mathbb{C}(\varepsilon(u) - p)$. The discrete version (P_h) reads: Seek $(u_h, p_h, a_h) \in H_h \times L_h$ satisfying (3.4) for $\sigma_h := \mathbb{C}(\varepsilon(u_h) - p_h)$ and, for all $(q_h, b_h) \in L_h$,

$$(\sigma_h; q_h - p_h) + (a_h; b_h - a_h) \leq \int_{\Omega} j^*(q_h; b_h) \, d\Omega - \int_{\Omega} j^*(p_h; a_h) \, d\Omega. \tag{3.13}$$

Theorem 5. The problem (P) (resp. (P_h)) is equivalent to (2.1) (resp. (2.2)) provided $\mathcal{K} = X = H \times L$ (resp. $\mathcal{K}_h = H_h \times L_h \subseteq \mathcal{K}$) and, for $x = (u, p, a), y = (v, q, b) \in X$

$$a(x; y) = (p - \varepsilon(u); \mathbb{C}(q - \varepsilon(v))) + (a; \mathbb{H}b),$$

$$\ell(y) = (f; v) + \int_{\Gamma_N} g \cdot v \, ds,$$

$$\psi(y) = \int_{\Omega} j^*(q, b) \, d\Omega.$$

Proof. Standard arguments (such as integration by parts) verify the assertion. \square

A second conclusion of Theorems 1 and 2 reads analogous to Theorem 4.

Theorem 6. *Let (u, p, a) solve (P) and (u_h, p_h, a_h) solve (P_h) . Then,*

$$\|(u - u_h, p - p_h, a - a_h)\|_{H \times L} \leq c_6(\eta_Z + \|[h_\epsilon^{3/2} \partial_\epsilon g / \partial s]\|_{L^2(\Gamma_N)} + \|h_{\mathcal{T}} \nabla f\|_{L^2(\Omega)}). \tag{3.14}$$

The constant $c_6 > 0$ depends on the shape of the elements (minimum angle condition), on the material parameters and on the type of hardening or viscoplastic regularisation.

Proof. The beginning follows the arguments of the proof of Theorem 4 and the definition of (q_h, b_h) as integrals means of (p, a) . Theorem 2 and the remaining arguments for the proof (3.9) yield in the present case that

$$\begin{aligned} c_7 \|(\sigma - \sigma_h, a - a_h)\|_L^2 &\leq (p_h - \epsilon(v_h); \mathbb{C}\epsilon(u - u_h)) + (f; u - v_h) + \int_{\Gamma_N} g \cdot (u - v_h) \, ds \\ &= -(\sigma_h; \epsilon(e - e_h)) + (f; e - e_h) + \int_{\Gamma_N} g \cdot (e - e_h) \, ds \end{aligned} \tag{3.15}$$

for $\sigma_h = \mathbb{C}(\epsilon(u_h) - p_h)$ and e, e_h as in the proof of Theorem 4. The arguments which led to (3.10) and (3.11) apply to (3.15) as well and eventually conclude the proof of (3.14). \square

4. Examples in elastoplasticity with hardening and viscoplastic regularisation

This section is devoted to list a few material functions j and j^* which arise in (3.3) and (3.12), respectively. It is discussed whether (i.e., for hardening or viscoplasticity) or not (i.e., for perfect plasticity) the conditions of Theorems 4 and 6 are satisfied.

In all the following cases, the functional j is defined as the characteristic functional of the (varying) admissible set \mathcal{K} , i.e.,

$$j(\tau, \beta) = \begin{cases} 0 & \text{if } (\tau, \beta) \in \mathcal{K}, \\ \infty & \text{if } (\tau, \beta) \notin \mathcal{K}. \end{cases} \tag{4.1}$$

The set \mathcal{K} is described by a yield function Φ as $\mathcal{K} = \{(\tau, \beta) \in \mathbb{R}_{\text{sym}}^{d \times d} \times \mathbb{R}^m \mid \Phi(\tau, \beta) \leq 0\}$.

4.1. Isotropic hardening

Let $m = 1$, i.e., α is a (non-negative) scalar, and define

$$\Phi(\sigma, \alpha) := |\text{dev } \sigma| - \sigma_y(1 + H\alpha) \tag{4.2}$$

in case $\alpha \geq 0$ (and $\Phi(\sigma, \alpha) = \infty$ if $\alpha < 0$ which, thereby, is not allowed). With the trace $\text{tr } A := \sum_{j=1}^d A_{jj}$ and the $d \times d$ -unit matrix I_d , the deviatoric part of a matrix $A \in \mathbb{R}^{d \times d}$ is

$$\text{dev } A := A - \frac{1}{d}(\text{tr } A)I_d.$$

The material constant $\sigma_y > 0$ is the yield stress and the constant $H > 0$ is the modulus of hardening. Then, there exists a unique solution of (P) provided the exterior load f is slightly more regular (and then there holds Johnson’s safe-load assumption) [15, 16]. The dual functional is known (see, e.g., [6] for a proof); for all $A \in \mathbb{R}_{\text{sym}}^{d \times d}$ and $B \in \mathbb{R}$,

$$j^*(A, B) = \begin{cases} \sigma_y |A| & \text{if } \operatorname{tr} A = 0 \wedge B + H\sigma_y |A| \leq 0, \\ \infty & \text{if } \operatorname{tr} A \neq 0 \vee B + H\sigma_y |A| > 0. \end{cases} \tag{4.3}$$

4.2. Kinematic hardening

Let $m = d(d + 1)/2$ and identify $\mathbb{R}^m \equiv \mathbb{R}_{\text{sym}}^{d \times d} := \{A \in \mathbb{R}^{d \times d} : A = A^T\}$. Like the stress σ we consider α (pointwise) as a $\mathbb{R}_{\text{sym}}^{d \times d}$ -matrix and define

$$\Phi(\sigma, \alpha) := |\operatorname{dev} \sigma - \operatorname{dev} \alpha| - \sigma_y. \tag{4.4}$$

Then, there exists a unique solution of (P) provided the exterior load f is slightly more regular (and then there holds Johnson’s safe-load assumption) [14–16]. The dual functional equals (see, e.g., [6] for a proof), for all $A, B \in \mathbb{R}_{\text{sym}}^{d \times d}$,

$$j^*(A, B) = \begin{cases} \sigma_y |A| & \text{if } \operatorname{tr} A = 0 \wedge B = -A, \\ \infty & \text{if } \operatorname{tr} A \neq 0 \vee B \neq -A. \end{cases} \tag{4.5}$$

4.3. Combined isotropic and kinematic hardening

Let $m = 1 + d(d + 1)/2$, identify $\mathbb{R}^m \equiv \mathbb{R} \times \mathbb{R}_{\text{sym}}^{d \times d}$, and write $\alpha = (a, b)$. Define

$$\Phi(\sigma, a, b) := |\operatorname{dev} \sigma - \operatorname{dev} b| - \sigma_y(1 + Ha) \tag{4.6}$$

in case $a \geq 0$ (and $\Phi(\sigma, \alpha) = \infty$ if $a < 0$ which, thereby, is not allowed). Then there exists a unique solution of (P) provided the exterior load f is slightly more regular (and then there holds Johnson’s safe-load assumption) [14]. The dual functional equals (see, e.g., [8] for a proof), for all $A \in \mathbb{R}_{\text{sym}}^{d \times d}$ and $B = (a, b) \in \mathbb{R} \times \mathbb{R}_{\text{sym}}^{d \times d}$

$$j^*(A, B) = \begin{cases} \sigma_y |A| & \text{if } \operatorname{tr} A = 0 \wedge b = -A \wedge a + \sigma_y H |A| \leq 0, \\ \infty & \text{if } \operatorname{tr} A \neq 0 \vee b \neq -A \vee a + \sigma_y H |A| > 0. \end{cases} \tag{4.7}$$

Furthermore, if $(\sigma, \chi) \in \partial j^*(p, \xi)$ and $\chi = (a, b)$, $\xi = (\alpha, \beta) \in \mathbb{R} \times \mathbb{R}_{\text{sym}}^{d \times d}$ such that $p \neq 0$, then

$$\frac{\operatorname{dev}(\sigma - b)}{\sigma_y(1 + Ha)} = p/|p| \quad \text{and} \quad \alpha = -\sigma_y H |p|. \tag{4.8}$$

4.4. Perfect plasticity

In the case $m = 0$ of no hardening, i.e., the internal variables are absent, the yield function reads

$$\Phi(\sigma) := |\operatorname{dev} \sigma| - \sigma_y. \tag{4.9}$$

The resulting problem is covered in this section, but the missing hardening leads to a different functional analytic frame. There exist solutions of (P) in a much weaker sense (space of bounded deformation $\text{BD}(\Omega)$) if Johnson’s safe-load assumption holds [28,29]. For any $A \in \mathbb{R}_{\text{sym}}^{d \times d}$, let $j^*(A) = \sigma_y |A|$ if $\operatorname{tr} A = 0$ and otherwise $j^*(A) = \infty$.

4.5. Viscoplasticity

In Examples 4.1, 4.2, and 4.4 the functional (4.1) is non-smooth, but may be approximated by a smoother functional. The Yosida regularisation leads to a viscoplastic material description in the sense of Perzyna where, given a viscosity $\mu > 0$, for all preceding examples of Φ we define

$$j(\sigma, \alpha) := \frac{1}{2\mu} \inf\{ |(\sigma - \tau, \alpha - \beta)|^2 : (\tau, \beta) \in \mathbb{R}_{\text{sym}}^{d \times d} \times \mathbb{R}^m \text{ with } \Phi(\tau, \beta) \leq 0 \}. \tag{4.10}$$

For $\mu > 0$ there exists a unique solution of Problem (P) [28]. The dissipation functional (4.10) is, in some sense, converging towards (4.1) as $\mu \rightarrow 0$ [28]. Some calculations verify formulae for the dual functional, e.g., in perfect plasticity of Example 4.4, we obtain

$$j^*(A) = \begin{cases} \sigma_y |A| + \frac{\mu}{2} |A|^2 & \text{if } \text{tr} A = 0, \\ \infty & \text{if } \text{tr} A \neq 0. \end{cases} \tag{4.11}$$

According to $\mu > 0$, the functional analytical frame of this paper is applicable (but not for $\mu = 0$).

5. Numerical examples

This section reports on numerical experiments on a posteriori error control and adaptive mesh-refining in practice. All the discretisations are generated by Algorithm 1 where $\Theta = 0$ for uniform meshes (as all elements in step (e) are marked) and $\theta = 1/2$ for adaptive mesh-refining (related strategies and a different choice for $0 < \Theta < 1$ are disputable).

Algorithm 1

- (a) Start with a coarse mesh \mathcal{T}_0 , set $k = 0$.
- (b) Solve the discrete problem with respect to the actual mesh \mathcal{T}_k for N degrees of freedom.
- (c) Compute $\eta_T = \eta_{T,Z}$ (resp. $\eta_T = \eta_{T,R}$) for all $T \in \mathcal{T}_k$.
- (d) Compute $\eta_N := (\sum_{T \in \mathcal{T}} \eta_T^2)^{1/2}$ as an estimate for the stress error $e_N := \|\mathbb{C}^{-1/2}(\sigma - \sigma_h)\|_{L^2(\Omega)}$.
- (e) Mark the element T for (*red*) refinement provided

$$\Theta \max_{K \in \mathcal{T}_k} \eta_K \leq \eta_T.$$

- (f) Mark further elements (within a *red-green-blue* refinement) to avoid hanging nodes. Define the resulting mesh as the actual mesh \mathcal{T}_{k+1} , update k and go to (b).

Details on the so-called *red-green-blue* refinement strategies may be found in [30]. We employed the ZZ-type average operator \mathcal{A} to define $\sigma_h^* := \mathcal{A}\sigma_h$ for which $\mathcal{A}\sigma_h(z)$ is the integral mean of (all components of) σ_h over the patch of z plus interpolation properties according to (1.8) [11].

Three different subsections include the three examples presented with focus on the performance of the error e_N and the two error estimators η_N (from (1.6) and (1.7) resp. (1.4) and (1.5)) as a function of the degrees of freedom N .

5.1. Elastoplastic ring with known solution

The first example involves kinematic hardening for the geometry shown in Fig. 1 which represents a ring with inner radius 1 and an outer radius of 2. We have no volume force ($f = 0$) but radially applied surface forces $g_1(r, \phi, t) = te_r$ and $g_2(r, \phi, t) = -t/4e_r$, $e_r = (\cos \phi, \sin \phi)$.

The analytical solution for a body centred at the origin with no rotation reads

$$u(r, \phi, t) = u_r(r, t)e_r, \tag{5.1}$$

$$\sigma(r, \phi, t) = \sigma_r(r, t)e_r \otimes e_r + \sigma_\phi(r, t)e_\phi \otimes e_\phi, \tag{5.2}$$

$$p(r, \phi, t) = p_r(r, t)(e_r \otimes e_r - e_\phi \otimes e_\phi), \tag{5.3}$$

(see [1] for details) with $e_\phi = (-\sin \phi, \cos \phi)$ and

$$\begin{aligned} u_r(r, t) &= \frac{t}{2\mu r} - \frac{2}{3}\kappa(r + 4a/(\mu r))I(1) - 2\kappa r I(r), \\ \sigma_r(r, t) &= -\frac{t}{r^2} - \frac{2}{3}a\kappa(1 - 4/r^2)I(1) - 2a\kappa I(r), \\ \sigma_\phi(r, t) &= \partial(r \cdot \sigma_r)/\partial r, \\ p_r(r, t) &= -\frac{\sigma_y}{\sqrt{2}(a\kappa + \mathbb{H})}(R^2/r^2 - 1)_+, \\ I(r) &= -\frac{\sigma_y}{\sqrt{2}(a\kappa + \mathbb{H})} \left[\frac{1}{2}(R^2/r^2 - 1)_+ - (\ln(R/r))_+ \right]. \end{aligned}$$

The radius of the circular plastic boundary $R(t)$ is determined by $\alpha \ln R^2 = (\alpha - 1)R^2 - \alpha + (\sqrt{2}/\sigma_y)t$. For material parameters from Fig. 1, the inner part of the body becomes plastic at $t = 171.8269$. We realised the time-increment from $t_0 = 0$ to $t_1 = 310$. (cf. [2, Example 1] for a justification of this huge time-step.)

According to symmetry, only a quarter of the domain is discretised with symmetric boundary conditions and the coarse mesh \mathcal{T}_0 consisting of three triangles as shown in Fig. 1. Within each refinement step (f) of Algorithm 1, new nodes on the boundary are projected onto the curved boundary.

Fig. 2 shows the true error e_N (marked by continuous lines) and the estimated errors η_Z (marked by dashed lines) and η_R (marked by dotted lines) from (1.6) to (1.7) and (1.4) to (1.5), respectively, versus the number N of degrees of freedom.

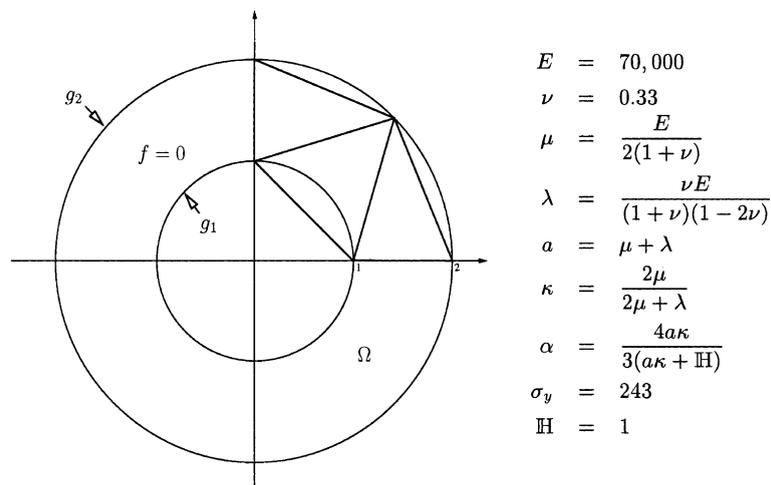


Fig. 1. Mechanical system and coarse mesh \mathcal{T}_0 in Example 5.1.

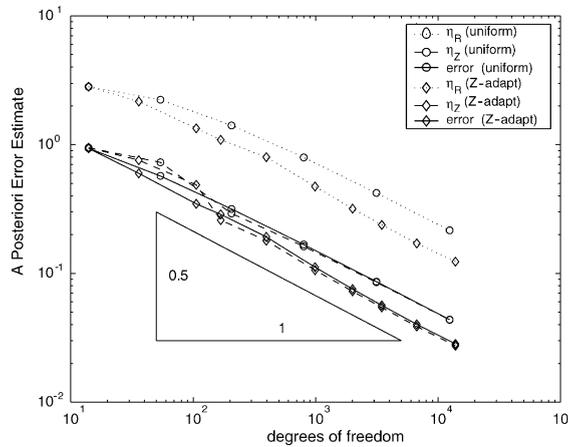


Fig. 2. True and estimated errors e_N, η_Z, η_R vs. N for Example 5.1.

The lines marked with circles result from uniform mesh-refinements (i.e., $\Theta = 0$ in Algorithm 1), the lines with the diamond-shaped markers are the results for an adaptive mesh-refinement (where $\Theta = 1/2$ in Algorithm 1) based on (1.4).

It is remarkable that, after some minor preasymptotic differences, the true error and the ZZ-estimator are practically identical while the residual-based estimate overestimates the true error by nearly constant factor 3. It should be mentioned that the estimators η_Z and η_R are reliable up to a constant C , i.e., $\|\sigma - \sigma_h\|_{L^2} \leq C\eta_Z$. The constant C depends on the shape of the elements as well as on the hardening parameters and so the use of $C = 1$ lacks a rigorous justification. (The use of $C = 1$ is justified as in [4,10,11] etc. by the efficiency estimate (1.10).)

The lacking improvement in the convergence-rate for the adaptive mesh refinement is not surprising because of the smoothness of the solution. The adaptively refined meshes show a slightly higher refinement at the curved boundary (cf., e.g., [3]).

5.2. L-shape

The second example is the L-shaped problem as shown in Fig. 3 with vanishing volume force f and Dirichlet boundary condition $u = u_D$ on Γ_D where $u_D := (u_r, u_\theta)$ is defined in polar coordinates by

$$u_r(r, \theta) = \frac{1}{2\mu} r^\alpha [-(\alpha + 1) \cos((\alpha + 1)\theta) + (C_2 - (\alpha + 1))C_1 \cos((\alpha - 1)\theta)],$$

$$u_\theta(r, \theta) = \frac{1}{2\mu} r^\alpha [(\alpha + 1) \sin((\alpha + 1)\theta) + (C_2 + \alpha - 1)C_1 \sin((\alpha - 1)\theta)].$$

For $\sigma_y = \infty$, i.e., for elastic material, (u_r, u_θ) is the analytical solution with a typical corner singularity in the stress variable at $(0, 0)$. In the elastoplastic case $\sigma_y = 2.2$, the exact solution is unknown but shows possibly a similar singularity at the origin. Hence adaptive algorithms should lead to a better convergence. The coarse mesh \mathcal{T}_0 consisted of six triangular elements as shown in Fig. 3 and we considered linear isotropic hardening.

In Fig. 4 the error estimates η_R and η_Z are compared with markers from Example 5.1.

The residual-based estimate η_R overestimates the ZZ-estimate η_Z by nearly a constant factor 4. The comparison with Example 5.1 led us to the conjecture that, in the present example, η_Z might be very close to the true (but unknown) error e_N . Fig. 4 further shows that the uniform mesh-refinement converges only

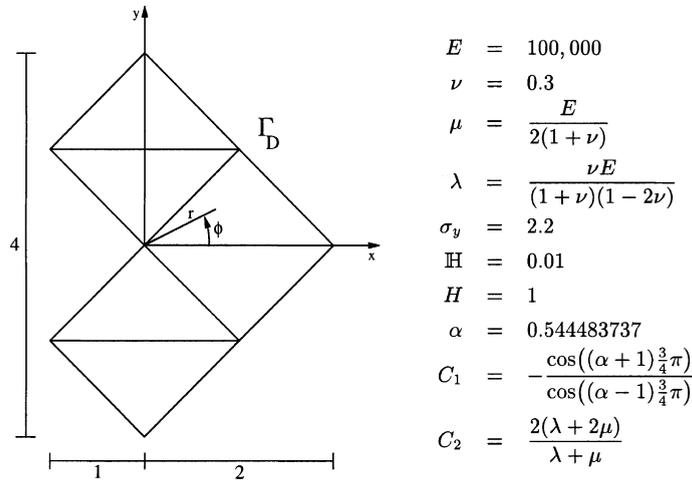


Fig. 3. Mechanical system and coarse mesh \mathcal{T}_0 in Example 5.2.

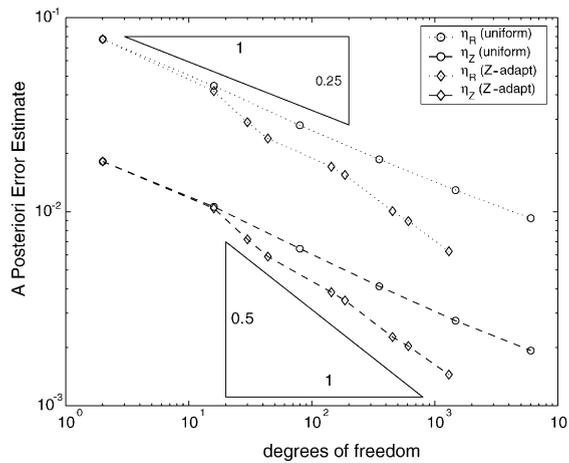


Fig. 4. Estimated errors η_Z and η_R vs. N for Example 5.2.

sub-optimally due to the singularity while the adaptive mesh-refinement yields optimal order of convergence. For the adaptively refined meshes, the algorithm of [3] showed problems in finding a solution beyond N plotted in Fig. 4. A possible explanation is that for the Newton–Raphson scheme global convergence is not guaranteed without damping [3].

5.3. Cooks membrane

Cook’s membrane problem serves as a third example visualised in Fig. 5, where a panel is clamped at one end and subjected to a shear load $g = (0, 1)$ along the opposite end (and vanishing volume force $f = 0$). Linear isotropic hardening moduli and the coarse mesh \mathcal{T}_0 are given in Fig. 5.

Fig. 6 compares the error estimates for the ZZ-estimator η_Z and for the residual-based estimator η_R . The estimate η_R is greater than η_Z by a constant factor 4 which suggests, when compared with the results from Example 5.1, that $\eta_Z \approx e$.

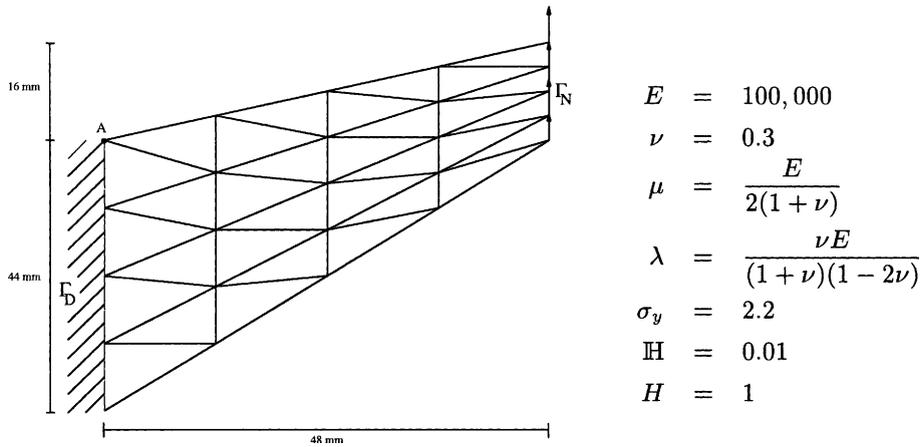


Fig. 5. Mechanical System and coarse mesh \mathcal{T}_0 in Example 5.3.

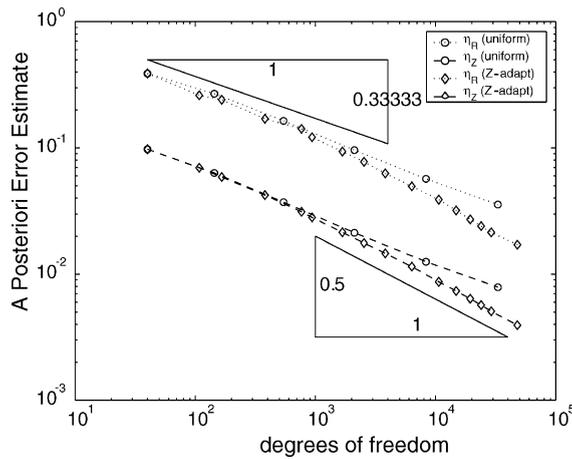


Fig. 6. Estimated errors η_Z and piecewise η_R vs. N for Example 5.3.

The proposed Algorithm 1 leads to a slightly better order of experimental convergence (at least of the upper bounds). The mesh is refined towards the point A in Fig. 5 where a change of the type of boundary conditions causes a singularity.

6. Conclusion

The mathematical justification of stress-averaging techniques for a posteriori error control is established for the primal and dual formulation of one time-increment in elastoplastic evolution by showing reliability and efficiency, i.e., we prove

$$\eta_Z^{(opt)} - \text{h.o.t.} \leq e \leq C_1 \eta_Z^{(opt)} + \text{h.o.t.}$$

for the minimal averaging estimate

$$\eta_Z^{(\text{opt})} := \min_{\sigma_h^* \in \mathcal{Q}(\mathcal{T}, g)} \|\mathbb{C}^{-1/2}(\sigma_h^* - \sigma_h)\|_{L^2(\Omega)}$$

on a continuous polynomial stress space $\mathcal{Q}(\mathcal{T}, g)$ that involves stress boundary conditions. Effective modifications of $\eta_Z^{(\text{opt})}$ are characterized (for a simpler model situation) in [9].

Conclusions from the *theoretical results* of this paper include:

- (i) Any stress-averaging estimator, such as any realisation of the ZZ-estimator is reliable.
- (ii) The estimator is the same as in linear elasticity although a different material law determines the stress approximation in elastoplasticity.
- (iii) The constant C_1 does neither depend on the number of degrees of freedom, the mesh-size, nor on the smoothness of the exact solution.
- (iv) The constant C_1 does depend on the domain, the shape of the elements (through their minimal angle).
- (v) The higher order terms in the upper bound (for reliability) depend on known data (such as ∇f and $\partial g/\partial s$), but not on (the questionable) higher regularity of the exact displacements.
- (vi) The higher order terms in the lower bound (for efficiency) depend on the smoothness of the stress field which is partly shown [25,26].
- (vii) The drawback of the reliability estimate is that C_1 depends crucially on the hardening moduli or viscosity. If corresponding parameters tend to zero, C_1 is expected to tend to infinity. In particular, the estimate is *not* justified in perfect plasticity.
- (viii) The estimate is true for constant material parameters such as \mathbb{C} and constant hardening moduli. For spatial-depending material laws, additional terms shall arise (cf., e.g., [8] for a corresponding involved analysis).

Conclusions from our *experimental results* include:

- (ix) The choice of the constant $C_1 = 1$ for practical error guess in the residual-based error estimator η_R overestimated the true stress error e_N by a factor between 3 and 4. This could be different (even worse) for different (e.g., smaller) hardening parameters.
- (x) The choice of the constant $C_1 = 1$ for practical error guess in the stress-average error estimator η_Z (motivated by $C_2 = 1$ in the efficiency estimate) leads to very good error predictions.
- (xi) It is conjectured that η_Z is a quite accurate error estimator which performs more accurate than our present mathematical analysis predicts.
- (xii) It seems not necessary to calculate the L^2 -projection of the finite element stress approximation σ_h to the space $\mathcal{Q}(\mathcal{T}, g)$ of feasible stress averages to compute $\eta_Z^{(\text{opt})}$. A simple local averaging to postprocess $\mathcal{A}\sigma_h$ suffices.
- (xiii) The adaptive mesh-refining Algorithm 1 proposed improves the quality of the spatial discretisation in case of non-optimal quasiuniform meshes. At least the related estimator η_Z but also the other η_R showed a significantly improved experimental convergence rate in those cases.

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