Three-field mixed finite element formulations for gradient elasticity at finite strains

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Abstract
Gradient elasticity formulations have the advantage of avoiding geometry-induced singularities and corresponding mesh dependent finite element solution as apparent in classical elasticity formulations. Moreover, through the gradient enrichment the modeling of a scale-dependent constitutive behavior becomes possible. In order to remain $C^0$ continuity, three-field mixed formulations can be used. Since so far in the literature these only appear in the small strain framework, in this contribution formulations within the general finite strain hyperelastic setting are investigated. In addition to that, an investigation of the inf sup condition is conducted and unveils a lack of existence of a stable solution with respect to the $L^2$-$H^1$-setting of the continuous formulation independent of the constitutive model. To investigate this further, various discretizations are analyzed and tested in numerical experiments. For several approximation spaces, which at first glance seem to be natural choices, further stability issues are uncovered. For some discretizations however, numerical experiments in the finite strain setting show convergence to the correct solution despite the stability issues of the continuous formulation. This gives motivation for further investigation of this circumstance in future research. Supplementary numerical results unveil the ability to avoid singularities, which would appear with classical elasticity formulations.

KEYWORDS
higher order gradients, mixed finite elements, nonlinear gradient elasticity

1 | INTRODUCTION

The internal elastic free energy density of classical hyperelastic formulations is a function of the first-order gradient of deformation. Although well established and sufficient for a broad spectrum of applications, these formulations have limitations when it comes to specific problems. For example, if the body of interest has a nonsmooth geometry such as sharp corners, the occurrence of non-physical stress singularities is possible and will lead to a pathological mesh dependency of corresponding finite-element simulations. The gradient elasticity approach can represent a remedy in these cases. Through enrichment of second-order deformation gradients into the internal elastic energy, the smoothness of the corresponding solution is increased and before mentioned geometry-induced singularities are avoided. Consequently, associated finite-element simulations remain mesh-objective.\cite{1-3}
Another field of application is the modeling of very small structures. When the specimen of interest reaches a microscopic size, the influence of the microstructure on the constitutive behavior becomes significant. These so-called size-effects cannot be modeled by classical local elasticity formulations. While molecular or even atomistic models can be used to capture these effects, corresponding simulations, however, quickly reach their computational limits, when the modeled nanostructure is more complex. Gradient elasticity formulations on the other hand capture the size effects through additional constitutive parameters imposed in the gradient enriched term of the elastic energy. Compared to atomistic models they are computationally much cheaper. Examples of the simulation of size-effects with a focus on the general formulation and numerical aspects can be found in Askes et al.\cite{2, 4, 5} while investigations of gradient elasticity approaches with a focus on specific applications can be found in Aifantis et al.\cite{6–10} Another application of gradient elasticity approaches is the unstable elastic energy of domains with martensitic phase transformations.\cite{12, 3, 11}

Significant theoretical foundations of these various applications date back to the 1960s gradient enriched elastic continuum theories with notable works of Mindlin\cite{12} and Toupin\cite{13, 14}. A noteworthy adaptation which proved to be a simplified special case of Mindlin’s theory was established by Aifantis.\cite{15} For a comprehensive historical overview the reader is referred to Askes and Aifantis.\cite{2} The idea of gradient enrichment for elasticity problems gave also rise to numerous gradient enriched plasticity models (cf. Aifantis et al.\cite{4, 16, 17} amongst others) and also to approaches for the regularization of damage formulations through gradient enrichment (cf. de Borst et al.\cite{18, 19} amongst others). Investigations with respect to evaluation of constitutive gradient elasticity constants are undertaken in Peerlings and Fleck.\cite{20} While most of the gradient elasticity models are restricted to the regime of small strains, investigations of gradient elastic constitutive models for large deformations can be found in Behesht\cite{21} and Triantafyllidis et al.\cite{22} 

Despite its before mentioned advantages over classical formulations, gradient elasticity formulations have not found a significant employment in general practical applications yet. One reason for this is a difficult numerical implementation due to their higher continuity requirements for corresponding finite element formulations. While the underlying equations of classical formulations are partial differential equations of second order, the corresponding equations of gradient elasticity formulations are of fourth order. Thus, discrete weak forms of classical elasticity formulations require \( C^0 \)-continuous interpolating functions, while gradient elasticity formulations require \( C^1 \)-continuous interpolations, whose numerical implementation, especially in the finite element framework is not straightforward.

An investigation of meshless discretization methods for the gradient elasticity formulation can be found in Askes and Aifantis\cite{15, 23} whereas in Papanicolopulos et al.\cite{24} a \( C^1 \)-continuous finite element with a preprocessing smoothing based on a least squared minimization is presented. The drawback of the latter one is the restriction to structured meshes only. The works of Rudraraju et al.\cite{3, 11} consider isogeometric analysis (IGA) as discretization scheme. Although the realization of the \( C^1 \)-continuity condition is straightforward in IGA, the well-known difficulties of meshing more complex structures and boundary conditions remain a research challenge.

Alternatively, by deriving mixed gradient elasticity formulations, standard \( C^0 \)-continuous finite element approximation schemes can be obtained. Based on the idea of Ru et al.\cite{25} in which the fourth-order gradient elasticity problem of Aifantis\cite{15} is split into two second order problems, a \( C^0 \)-continuous corresponding finite element formulation is possible.\cite{26} While the latter is restricted to the special formulation of Aifantis\cite{15} in Shu et al.\cite{27} and Zybell\cite{28} a mixed approach is investigated, which enables \( C^0 \)-continuous discretizations in the framework of the more general Mindlin-Toupin gradient elasticity theory.

The mixed approaches of Shu et al.\cite{27} and Zybell\cite{28} are promising with respect to their use in commercial software, because corresponding discrete forms are conform with well established standard finite element schemes, that is, the modeled structures can be arbitrarily complex since associated meshing procedures are available. However, due to the introduction of additional discretization variables, the computational cost is relatively high. Moreover, a mathematical analysis with respect to stability and the extension of specific formulations to nonlinear problems are still missing in the literature. This is the starting point of the present contribution, in which three-field mixed finite element formulations are proposed for the general nonlinear hyperelastic framework. These are then mathematically and numerically investigated with respect to stability.

In Section 2 a continuum mechanical overview of the gradient elasticity theory is given, followed by the introduction of the continuous three-field formulation for finite strains in Section 3 together with stability considerations in Section 4. The discretization procedure for the corresponding finite element formulations and the stability investigations of various approximations are given in Section 5. In Section 6 numerical examples are presented and a conclusion is given in Section 7.
2 | CONTINUUM MECHANICAL FRAMEWORK

2.1 | Notation

For $\mathcal{M} = \mathbb{R}$, $\mathbb{R}^d$ or $\mathbb{R}^{d \times d}$, the space of tensor-valued functions whose components are square integrable over a body $B$ is denoted by $L^2(B; \mathcal{M})$. The corresponding $L^2$-inner product and the $L^2$-norm for any tensor function $v$

$$\langle \delta v, v \rangle_{L^2(B)} := \int_B \delta v \cdot v \, dV \quad \text{and} \quad \|v\|_{L^2(B)} := \sqrt{\int_B v \cdot v \, dV}. \quad (2.1)$$

Let $\text{Curl}$ denote the Curl-operator, that is

$$\text{Curl} v = \left( \frac{\partial v}{\partial x} \right)_{d=2} \quad \text{and} \quad \text{Curl} v = \left( \frac{\partial v_3}{\partial x} - \frac{\partial v_2}{\partial y} \right)_{d=3}$$

and let $\wedge$ denote the cross product. For vector or tensor valued functions, the operators $\nabla$, $\text{div}$ and $\text{Curl}$ are applied row-wise. The cross product $\wedge : \mathbb{R}^{3 \times 3} \times \mathbb{R}^3 \to \mathbb{R}^{3 \times 3}$ acts on tensor fields as

$$(a \wedge b)_{i,1} := a_{i,2}b_3 - a_{i,3}b_2,$$

$$(a \wedge b)_{i,2} := -a_{i,1}b_3 + a_{i,3}b_1,$$

$$(a \wedge b)_{i,3} := a_{i,1}b_2 - a_{i,2}b_1$$

for $i \in \{1, 2, 3\}$. Let $H^1(B; \mathcal{M})$ denote the Sobolev space of $L^2$-functions with gradient in $L^2$ and let $H^1_0(B; \mathcal{M})$ denote the space of $H^1(B; \mathcal{M})$ functions with vanishing trace, that is, $v|_{\partial B} = 0$. Furthermore, define

$$H(\text{Curl}, B; \mathbb{R}^{3 \times 3}) := \{ v \in L^2(B; \mathbb{R}^{3 \times 3}) : \text{Curl} v \in L^2(B; \mathbb{R}^{3 \times 3}) \},$$

$$H_0(\text{Curl}, B; \mathbb{R}^{3 \times 3}) := \{ v \in H(\text{Curl}, B; \mathbb{R}^{3 \times 3}) : (v \wedge n)|_{\partial B} = 0 \},$$

$$H(\text{div}, B; \mathbb{R}^{3 \times 3}) := \{ v \in L^2(B; \mathbb{R}^{3 \times 3}) : \text{div} v \in L^2(B; \mathbb{R}^3) \}$$

wherein $n$ denotes the unit vector normal to $\partial B$.

2.2 | Kinematic fundamentals

Let the bounded Lipschitz domain $B \subseteq \mathbb{R}^d : d \in \{2, 3\}$ be the body of interest in the reference configuration and $S \subseteq \mathbb{R}^d : d \in \{2, 3\}$ be the body in the current configuration. For each material point defined by the position vector $X \in B$ in the reference configuration there exists a corresponding position vector $x \in S$ in the current configuration defined by the deformation map $\varphi : B \to S$. The deformation map can be described by $\varphi(X, t) = X + u(X, t)$ in terms of the displacement function $u$.

Denote $\nabla(\bullet) = \partial(\bullet)/\partial X$ as the gradient of a vector-/tensor-valued function with respect to the position vector in the reference configuration. The deformation gradient is written as

$$F = \nabla \varphi = I + \nabla u \quad (2.2)$$

with $I$ denoting the identity tensor of second order.

2.3 | Gradient elasticity theory

According to the gradient elasticity theory,[12,14] the boundary of $B$ can be decomposed in the following way:

$$\partial B = \Gamma_D \cup \Gamma_N = \Gamma_H \cup \Gamma_M \quad \text{and} \quad \Gamma_D \cap \Gamma_N = \Gamma_H \cap \Gamma_M = \emptyset, \quad (2.3)$$
with \( \Gamma_D \) and \( \Gamma_N \) being the standard Dirichlet- and Neumann boundaries, respectively, and \( \Gamma_H \) and \( \Gamma_M \) being Dirichlet- and Neumann boundaries on which higher-order quantities are prescribed. The hyperelastic strain energy density, which in classical formulations is a function of the deformation gradient, is enriched by a dependency on the second-order deformation gradient, that is

\[
W := W(F) \quad \text{(classical elasticity)} \quad \Rightarrow \quad W := W(F, \nabla F) \quad \text{(gradient elasticity)}.
\]  

In order to retain frame invariance, the preferred choice for the non-gradient enriched elastic energy density are functions \( W := W(C) \), which can be expressed in terms of the right Cauchy tensor \( C = F^T F \). Corresponding investigations with respect to frame invariance of the gradient enriched elastic energy can be found in Triantafyllidis and Aifantis\cite{Triantafyllidis2018} and will be taken up in Section 6.

Denote \( D(\bullet) = \nabla(\bullet) \cdot n \) as the derivative in normal direction \( n \) defined on the surface \( \partial B \). The gradient elasticity boundary value problem can be formulated as the minimization problem

\[
\Pi[\bar{u}] = \int_B W(F(\bar{u}), \nabla F(\bar{u})) \, dV + \Pi^{\text{ext}} \Rightarrow \min_{\bar{u}} \Pi[\bar{u}],
\]

\[
\text{with} \quad \Pi^{\text{ext}}[\bar{u}] = -(\bar{u}, f)_{L^2(B)} - \int_{\Gamma_N} \bar{u} \cdot t \, dA - \int_{\Gamma_M} \bar{D} \cdot r \, dA,
\]

where \( \Pi^{\text{ext}} \) is the external potential of volume load \( f \), surface traction \( t \) and surface moment\(^1\) \( r \), which is work conjugated to the displacement gradient \( \bar{D} \bar{u} \) in normal direction. The minimizer \( u \), for which \( d\Pi[\bar{u}] / d\varepsilon|_{\varepsilon=0} = 0 \) holds with \( \bar{u} = u + \varepsilon \delta u \) is sought in

\[
u \in H^2(B; \mathbb{R}^d) \quad \text{with} \quad u = \bar{u} \text{ on } \Gamma_D \quad \text{and} \quad D\!u = \bar{h} \text{ on } \Gamma_H,\]

where the essential boundary conditions consist of prescribed displacements \( \bar{u} \) and prescribed displacement gradients in normal direction \( \bar{h} \). Because of the affiliation to \( H^2 \), corresponding discrete functions of \( \bar{u} \) have the requirement to be \( C^1 \)-continuous, for which the design and implementation of conforming finite elements is not straightforward.

### 3 | THREE-FIELD MIXED FORMULATION

In order to arrive at a formulation, which enables \( C^0 \)-continuous discretizations, a mixed three-field approach is considered. Based on the three-field potential for small strains given in Shu et al.,\cite{Shu2016} we propose an associated formulation for finite strains as

\[
P[\bar{u}, \bar{H}, \bar{\lambda}] = \int_B W(F(\bar{u}), \nabla F(\bar{H})) \, dV + (\bar{\lambda}, \bar{H} - \nabla \bar{u})_{L^2(B)} + \Pi^{\text{ext}}.
\]

Here, in the gradient enriched part of \( W, \nabla u \) is replaced by the new independent variable \( H \in H^1(B; \mathbb{R}^{d \times d}) \) and compatibility is enforced in an integral sense via Lagrange multiplier \( \lambda \in L^2(B; \mathbb{R}^{d \times d}) \). The introduction of \( H \) enables a relaxation of the continuity requirement to \( C^0 \). We introduce

\[
P := \frac{\partial W}{\partial F} \quad \text{and} \quad G := \frac{\partial W}{\partial \nabla F}
\]

where \( P \) is known as the first Piola Kirchhoff stress tensor and \( G \) denotes a higher order stress tensor. Consequently, the variational equation

\[
\delta_u \Pi = (\nabla \delta u, P)_{L^2(B)} - (\nabla \delta u, \lambda)_{L^2(B)} - (\delta u, f)_{L^2(B)} - \int_{\Gamma_N} \delta u \cdot t \, dA = 0
\]

\[
\delta_H \Pi = (\nabla \delta H, G)_{L^2(B)} + (\delta H, \lambda)_{L^2(B)} - \int_{\Gamma_M} (\delta H \cdot n) \cdot r \, dA = 0
\]

\[
\delta_\lambda \Pi = (\delta \lambda, H - \nabla u)_{L^2(B)} = 0
\]

\(^1\)Varying denotations for \( r \) appear in the literature. In, for example, Shu et al.,\cite{Shu2016} \( r \) is named higher order stress traction.
is obtained. For the mathematical analysis we consider the small strain setting and investigate the analogous formulation to (3.3) to (3.5) with \( \partial \mathcal{B} = \Gamma_D = \Gamma_H \) for the special case of quadratic local and nonlocal strain energies. Given \( f \in L^2(B; \mathbb{R}^2) \) find \( u \in H^1_0(B; \mathbb{R}^d) \) with

\[
\kappa(\nabla^2 u, \nabla^2 \delta u)_{L^2(B)} + (\mathbb{C} e(u), e(\delta u))_{L^2(B)} = (f, \delta u)_{L^2(B)} \quad \text{for all } \delta u \in H^1_0(B; \mathbb{R}^d). \tag{3.6}
\]

Herein, \( \kappa \) denotes a material parameter associated with the higher-order stress response, \( \mathbb{C} \) is the elasticity tensor of fourth order for linear elasticity, and \( e \) denotes the linear strain tensor. Thereby, an energy function is considered which is additionally split into a local (classical) quadratic part depending on \( e \) and a nonlocal quadratic part depending on \( \nabla u \).

The corresponding mixed formulation seeks \((u, H, \lambda) \in H^1_0(B; \mathbb{R}^d) \times H^1_0(B; \mathbb{R}^{d \times d}) \times L^2(B; \mathbb{R}^{d \times d})\) with

\[
a((u, H), (\delta u, \delta H)) + B((\delta u, \delta H), \lambda) = (f, \delta u)_{L^2(B)},
\]

\[
B((u, H), \delta \lambda) = 0 \quad \text{for all } \delta u, \delta H, \delta \lambda \in H^1_0(B; \mathbb{R}^d) \times H^1_0(B; \mathbb{R}^{d \times d}) \times L^2(B; \mathbb{R}^{d \times d}),
\]

where the bilinear forms \( a \) and \( B \) are defined by

\[
a((u, H), (\delta u, \delta H)) \triangleq \kappa(\nabla H, \nabla \delta H)_{L^2(B)} + (\mathbb{C} e(u), e(\delta u))_{L^2(B)},
\]

\[
B((\delta u, \delta H), \delta \lambda) \triangleq (\nabla \delta u, \delta \lambda)_{L^2(B)} - (\delta H, \delta \lambda)_{L^2(B)}
\]

for all \((u, H), (\delta u, \delta H) \in H^1_0(B; \mathbb{R}^d) \times H^1_0(B; \mathbb{R}^{d \times d})\) and \( \delta \lambda \in L^2(B; \mathbb{R}^{d \times d}) \).

### 4 Mathematical Analysis of the Continuous Formulation

This section analyzes the problem (3.7). It proves in Lemma 1 the equivalence of this problem with (3.6) in the sense that the solutions of the two problems coincide. However, problem (3.7) is not stable with respect to the standard norms \( \| (\bullet) \|_{H^1(B)}, \| (\bullet) \|_{H^1(B)} \) and \( \| (\bullet) \|_{L^2(B)} \) for the three variables \( u, H, \lambda \), respectively. This means that a small perturbation of the right-hand side, that is, the external potential, could lead to large deviations of the solutions in those norms. In particular, errors from, for example, numerical integration of the right-hand side could lead to large errors of the solution.

Since the bilinear form in (3.6) is continuous and coercive due to Poincaré’s inequality, Lax-Milgram yields existence of a unique solution. Poincaré’s inequality applied on \( \kappa(\nabla H, \nabla \delta H)_{L^2(B)} \) and a Korn’s inequality applied on \((\mathbb{C} e(u), e(\delta u))_{L^2(B)}\) show that the bilinear form \( a \) is coercive. Since the bilinear forms \( a \) and \( B \) are continuous, it would remain to prove an inf-sup condition to show that problem (3.7) is stable.

However, Proposition 1 shows that the inf-sup condition for the bilinear form (3.9) is not satisfied. Therefore the formulation (3.7) is not stable with respect to the standard norms and Brezzi’s splitting lemma does not guarantee the unique solvability.

**Proposition 1** Let \( d = 2, 3 \). Let \( B := [0, 1]^d \). There is no constant \( c > 0 \) such that for all \( \delta \lambda \in L^2(B; \mathbb{R}^{d \times d}) \)

\[
c \| \delta \lambda \|_{L^2(B)} \leq \sup_{(\delta u, \delta H) \in H^1_0(B; \mathbb{R}^d) \times H^1_0(B; \mathbb{R}^{d \times d})} \frac{B((\delta u, \delta H), \delta \lambda)}{\| \nabla \delta u \|_{L^2(B)} + \| \nabla \delta H \|_{L^2(B)}}. \tag{4.1}
\]

**Proof.** Let \( d = 2, 3 \), \( M = \mathbb{R}^2 \) for \( d = 2 \) and \( M = \mathbb{R}^{3 \times 3} \) for \( d = 3 \). Let \( \beta_n \in H^1_0(B, M) \) with \( \| \beta_n \|_{L^1(B)} = 1 \) be the sequence of eigenfunctions of the Laplace operator with corresponding eigenvalues \( \mu_1 \leq \mu_2 \leq \ldots \) with \( \mu_n \to \infty \) for \( n \to \infty \), that is,

\[
(\nabla \beta_n, \nabla \gamma)_{L^2(B)} = \mu_n (\beta_n, \gamma)_{L^2(B)} \quad \text{for all } \gamma \in H^1_0(B; M).
\]

Set \( \delta \lambda_n := \text{Curl} \beta_n \in L^2(B, \mathbb{R}^{d \times d}) \). Then \( \| \delta \lambda_n \|_{L^2(B)} = \sqrt{\mu_n} \) and

\[
B((\delta u, \delta H), \delta \lambda_n) = - (\delta \lambda_n, \delta H)_{L^2(B)} \leq \| \beta_n \|_{L^2(B)} \| \nabla \delta H \|_{L^2(B)} = \| \nabla \delta H \|_{L^2(B)}.
\]

Therefore \( \sup_{\delta H \in H^1_0(B; \mathbb{R}^{d \times d})} B((\delta u, \delta H), \delta \lambda_n)/(\| \nabla \delta H \|_{L^2(B)} + \| \nabla \delta u \|) \leq 1 = \| \delta \lambda_n \| / \sqrt{\mu_n}. \)

\[\blacksquare\]
The solution of (3.6) is for a suitable choice of \( H, \lambda \) a solution to (3.7) and vice versa.

**Lemma 1** If \( \mathbf{u} \) is the solution of (3.6), there exists \( (H, \lambda) \in H_0^1(B; \mathbb{R}^{d \times d}) \times L^2(B; \mathbb{R}^d) \) such that \( (u, H, \lambda) \) is a solution to (3.7). Conversely, if \( (\mathbf{u}, H, \lambda) \in H_0^1(B; \mathbb{R}^d) \times H^1_0(B; \mathbb{R}^{d \times d}) \times L^2(B; \mathbb{R}^{d \times d}) \) solves (3.7), then \( \mathbf{u} \) is in \( H_0^2(B; \mathbb{R}^d) \) and a solution to (3.6).

**Proof.** Let \( \mathbf{u} \) be the solution to (3.6). Let \( \mathbf{H} := \nabla \mathbf{u} \) and \( \lambda = 0 \). Then, \( B((\mathbf{u}, H), \delta \lambda) = 0 \) for all \( \delta \lambda \in L^2(B; \mathbb{R}^{d \times d}) \) and \( a((\mathbf{u}, H), (\delta \mathbf{u}, \delta H)) + B((\delta \mathbf{u}, \delta H), \lambda) = (f, \delta \mathbf{u})_{L^2(B)} \) for all \( (\delta \mathbf{u}, \delta H) \in H^1_0(B; \mathbb{R}^d) \times H^1_0(B; \mathbb{R}^{d \times d}) \). Conversely, let \( (\mathbf{u}, H, \lambda) \in H^1_0(B; \mathbb{R}^d) \times H^1_0(B; \mathbb{R}^{d \times d}) \times L^2(B; \mathbb{R}^{d \times d}) \) be the solution to (3.7). The choice \( \delta \lambda = \nabla \mathbf{u} - H \) implies \( B((\mathbf{u}, H), \delta \lambda) = \| \nabla \mathbf{u} - H \|_{L^2(B)}^2 = 0 \). Thus, \( \mathbf{H} = \nabla \mathbf{u} \) almost everywhere. Furthermore, \( \nabla \mathbf{u} = \mathbf{H} \in H^1_0(B; \mathbb{R}^{d \times d}) \) implies \( \mathbf{u} \in H^2_0(B; \mathbb{R}^d) \). Let \( \delta \mathbf{u} \in H^2_0(B; \mathbb{R}^d) \). With the choice \( \delta \mathbf{H} := \nabla \delta \mathbf{u} \in H^1_0(B; \mathbb{R}^{d \times d}) \) we obtain \( \kappa (\nabla^2 \mathbf{u}, \nabla^2 \delta \mathbf{u})_{L^2(B)} + (\mathbf{C} \mathbf{e}(\mathbf{u}), \mathbf{e}(\delta \mathbf{u}))_{L^2(B)} = a((\mathbf{u}, H), (\delta \mathbf{u}, \delta \mathbf{H})) = (f, \delta \mathbf{u})_{L^2(B)} \).

### 5 | FINITE ELEMENT FORMULATION

In the previous section it was shown that for the linear gradient elastic scenario at small strains stability with respect to the standard norms is not guaranteed. Since the investigation of continuity and coercivity of the nonlinear finite strain gradient elasticity problem (2.5) as well as applicability of Brezzi’s splitting lemma to the corresponding mixed problem (5.2) is not straightforward, analogous mathematical analysis of the constitutively and geometrically nonlinear formulation is left for future research. Nevertheless, similar problems with respect to stability are expected in the nonlinear regime. In order to investigate this, numerical analysis will be used. Thus, several large strain three-field finite element formulations are introduced in the following.

#### 5.1 | Discretization

In the following the general procedure for constructing the discrete system of equations is presented. The derivation of the corresponding matrices is here based on automatic differentiation (AD), which is increasingly used in finite element research as the development time is accelerated. For the finite element implementation and the numerical example computations, the software package AceGen/AceFEM has been used. Note that usage of AD is not required for the formulations discussed here and only applied as a technical tool.

Starting point for the discretization is the total potential (3.1). From the element partition of the continuum body it follows

\[
\Pi \approx \Pi^h = \sum_{e=1}^{n_e} \Pi^h_e.
\]

(5.1)

Subsequently, the discrete element potential takes the form

\[
\Pi^h_e = \int_{B_e} W(F(u_e^h), \nabla F(H_e^h)) \, dV + (\lambda^h_e, H_e^h - \nabla u_e^h)_{L^2(B_e)} + \Pi^\text{ext},h(u_e^h),
\]

(5.2)

where the solution variables are discretized with the continuous Galerkin method. They are based in finite dimensional subspaces \( V^h \subseteq V, \mathcal{G}^h \subseteq \mathcal{G} \) and \( Q^h \subseteq Q \) and can be written in matrix notation as

\[
\begin{align*}
\mathbf{u}^h_e &= N^u_e \mathbf{d}^u_e \quad \in \mathcal{V}^h, \\
H_e^h &= N^H_e \mathbf{d}^H_e \quad \in \mathcal{G}^h, \\
\lambda^h_e &= N^\lambda_e \mathbf{d}^\lambda_e \quad \in \mathcal{Q}^h,
\end{align*}
\]

(5.3)

where \( N^u_e, N^H_e \) and \( N^\lambda_e \) are standard matrices containing polynomial shape functions and \( \mathbf{d}^u_e, \mathbf{d}^H_e \) and \( \mathbf{d}^\lambda_e \) are vectors of the corresponding degrees of freedom associated with \( \mathbf{u}^h, H_e^h \), and \( \lambda^h \), respectively. The individual element degrees of freedom can be collected in the complete element vector of degrees of freedom of the discrete system as

\[
\mathbf{d}^e := [ (\mathbf{d}^u_e)^T \mid (\mathbf{d}^H_e)^T \mid (\mathbf{d}^\lambda_e)^T ]^T.
\]

(5.4)
The variation of (5.2) can then be written as

\[ \delta \Pi h = \sum_{e=1}^{n_e} \delta \Pi h^e [d_e] = 0, \quad \text{with} \quad \delta \Pi h = \delta d_e^T \frac{\partial \Pi h}{\partial d_e}, \]  

wherein \( \partial \Pi h / \partial d_e \) represents the element residual

\[ r_e = \left[ \begin{array}{c} (r^u_e)^T \\ (r^H_e)^T \\ (r^\lambda_e)^T \end{array} \right] := \left[ \begin{array}{ccc} \frac{\partial \Pi h}{\partial d_e^u} \\ \frac{\partial \Pi h}{\partial d_e^H} \\ \frac{\partial \Pi h}{\partial d_e^\lambda} \end{array} \right]^T. \]  

A detailed description of the individual residual components can be found in Appendix 7. For the numerical solution of the nonlinear problem \( A r_e = 0 \) using the Newton-Raphson procedure, the discrete variational equation (5.5) is linearized:

\[ \text{Lin} \left[ \delta \Pi h \right] = \sum_{e=1}^{n_e} \delta d_e^T \text{Lin} [r_e] = 0, \quad \text{with} \]

\[ \text{Lin} [r_e] = r_e (d_e) + \frac{\partial r_e}{\partial d_e} |_{d_e} \Delta d_e. \]

Herein, \( d_e \) represents the unknowns in the previous Newton iteration step, \( \Delta d_e \) depicts the linear increment of the nodal degrees of freedom and \( A \) is an appropriate assembly operator. Consequently, \( \frac{\partial r_e}{\partial d_e} \) represents the element tangent matrix

\[ k_e = \begin{bmatrix} k_e^{uu} & k_e^uH & k_e^{u\lambda} \\ k_e^{Hu} & k_e^HH & k_e^{H\lambda} \\ k_e^{\lambda u} & k_e^\lambda H & k_e^{\lambda\lambda} \end{bmatrix} := \frac{\partial r_e}{\partial d_e}. \]  

Again, a detailed description of the individual components of the tangent matrix is given in Appendix 7. Making use of the distributive property of the assembly operator yields the global system of equations

\[ \text{Lin} \left[ \delta \Pi h \right] = \delta D \cdot (R + K \cdot \Delta D) = 0, \quad \text{with} \]

\[ \delta D = \sum_{e=1}^{n_e} \delta d_e, \quad \Delta D = \sum_{e=1}^{n_e} \Delta d_e, \quad R = \sum_{e=1}^{n_e} r_e, \quad \text{and} \quad K = \sum_{e=1}^{n_e} k_e. \]  

All integrals are numerically evaluated with Gauss point integration over the isoparametric reference element. Note that with \( k_e^{HH} = (k_e^{Hu})^T = 0 \) and \( k_e^{\lambda\lambda} = 0 \) the global tangent matrix takes the form

\[ K = \begin{bmatrix} K_{uu} & 0 & K_{u\lambda} \\ 0 & K_{HH} & K_{H\lambda} \\ K_{u\lambda}^T & K_{H\lambda}^T & 0 \end{bmatrix}. \]  

5.2 Finite element approximations

In this section exemplary finite element approximations are investigated. For the discrete system, we consider partitions \( T \) of \( B \) into simplices. We define \( E, E(B), E(\partial B) \) to be the edges, the inner edges and the boundary edges of \( T \), respectively. We further define \( \mathcal{N}, \mathcal{N}(B), \mathcal{N}(\partial B) \) to be the nodes, the inner nodes and the boundary nodes of \( T \). We denote

\[ S_0^k(T; \mathbb{R}^{d^n}) := P_k(T; \mathbb{R}^{d^n}) \cap H^1_0(B; \mathbb{R}^{d^n}), \]  

(5.11)
where $P_k(T; \mathbb{R}^d)$ is the space of piecewise polynomial functions of degree $\leq k$ and $n$ is the tensorial order of the discretization variable. Consequently, $P_0(T; \mathbb{R}^d)$ is the space of piecewise constant functions. Table 1 shows an overview of the finite element pairs considered in the following.

### 5.2.1 Unstable discretizations

This section discusses several discretizations which, at first glance, seem to be natural choices. However, it will be shown that they are in fact not stable with respect to the norms considered in Section 4. Therefore, Brezzi’s splitting lemma\(^{[30]}\) proves that a unique discrete solution does not exist in general.

Lemma 2 proves that the P1-P1-P0 discretization in 2D is not stable.

**Lemma 2** Let $d = 2$ and $T$ be a regular triangulation into triangles. There exists a $\delta \lambda_h \in P_0(T; \mathbb{R}^{2\times 2})$ such that

$$0 = \sup_{(\delta u_h, \delta H_h) \in (S^1_0(T; \mathbb{R}^2) \times S^1_0(T; \mathbb{R}^{2\times 2}))} \frac{B((\delta u_h, \delta H_h), \delta \lambda_h)}{\|B(\delta u_h, \delta H_h)\|_{L^2(\Omega)} + \|\nabla \delta H_h\|_{L^2(\Omega)}}. \quad (5.12)$$

In particular, there exists in general no unique solution of (3.7) discretized with $(u_h, H_h, P_h) \in S^1_0(T; \mathbb{R}^2) \times S^1_0(T; \mathbb{R}^{2\times 2}) \times P_0(T; \mathbb{R}^{2\times 2})$.

**Proof.** Let $\delta u_h \in S^0_0(T; \mathbb{R}^2)$ and $\delta H_h \in S^0_0(T; \mathbb{R}^{2\times 2})$ be arbitrary. We define the Crouzeix-Raviart space

$$\text{CR}^1(T; \mathbb{R}^2) := \{ \beta_h \in L^2(B; \mathbb{R}^2) : \beta_h|_T \in P_1(T; \mathbb{R}^2) \text{ for all } T \in T \}$$

and the $T$-piecewise operator $\text{Curl}_h$ by $(\text{Curl}_h \beta_h)|_T := (\text{Curl} \beta_h)|_T$ for all $T \in T$ and $\beta_h \in \text{CR}^1(T; \mathbb{R}^2)$. The discrete Helmholtz decomposition\(^{[31]}\)

$$P_0(T; \mathbb{R}^{2\times 2}) = \nabla S^0_0(T; \mathbb{R}^2) \oplus \text{Curl}_h \text{CR}^1(T; \mathbb{R}^2) \quad (5.13)$$

(which is $L^2$-orthogonal) implies for any $\delta \lambda_h \in P_0(T; \mathbb{R}^{2\times 2})$ with $\delta \lambda_h := \text{Curl}_h \beta_h$ and $\beta_h \in \text{CR}^1(T; \mathbb{R}^2)$ that

$$B((\delta u_h, \delta H_h), \delta \lambda_h) = (\nabla \delta u_h, \text{Curl}_h \beta_h)_{L^2(\Omega)} - (\delta H_h, \text{Curl}_h \beta_h)_{L^2(\Omega)}.$$

The Euler-type formulae $2\#T + 1 = \#\mathcal{N} + \#E(B), \#E(B) + \#E = 3\#T$ and $E(\partial B) = \mathcal{N}(\partial B)$ imply $\#E = 3\#\mathcal{N} + \#\mathcal{N}(\partial B) - 3$ and we obtain

$$\dim(\text{Curl}_h(\text{CR}^1(T; \mathbb{R}^2))) = 2 \cdot (2\#\mathcal{N} + \#E(\partial B) - 3 - 1) > 2 \cdot 2\#\mathcal{N}(\partial B) = \dim S^1_0(T; \mathbb{R}^{2\times 2})$$

for all regular triangulations $T$. Thus there exists some $\beta_h \in \text{CR}^1(T; \mathbb{R}^2)$ with

$$(\delta H_h, \text{Curl}_h \beta_h)_{L^2(\Omega)} = 0 \quad \text{for all } \delta H_h \in S^1_0(T; \mathbb{R}^{2\times 2}).$$

The assertion follows with $\delta \lambda_h := \text{Curl}_h \beta_h \in P_0(T; \mathbb{R}^{2\times 2})$.

---

**Table 1** Summary of results of Section 5.2

| Element name | Discrete subspaces $V^h \times Q^h \times Q^h$ | Stability findings |
|--------------|---------------------------------------------|-------------------|
| P1-P1-P0 (2D) | $S^1_0(T; \mathbb{R}^2) \times S^1_0(T; \mathbb{R}^{2\times 2}) \times P_0(T; \mathbb{R}^{2\times 2})$ | Not stable |
| P2-P1-P1 (2D) | $S^1_0(T; \mathbb{R}^2) \times S^1_0(T; \mathbb{R}^{2\times 2}) \times P_0(T; \mathbb{R}^{2\times 2})$ | Stability depends on $h$ |
| Pk-P1-P0 (3D) | $S^0_0(T; \mathbb{R}^3) \times S^1_0(T; \mathbb{R}^{3\times 3}) \times P_0(T; \mathbb{R}^{3\times 3})$ | Not stable |
| P2-P1B-P0 (2D) | $S^2_0(T; \mathbb{R}^2) \times S^1_0(T; \mathbb{R}^{2\times 2}) \times P_0(T; \mathbb{R}^{2\times 2})$ | Stability depends on $B$ |
Lemma 3 proves that the Pk-P1-P0 discretization in 3D is not stable on any uniform triangulation \( T \) of \( B \cup \partial B = [0,1]^3 \) with nodes \( \mathcal{N} := \left\{ \left( \frac{i}{n}, \frac{j}{n}, \frac{k}{n} \right) : i, j, k \in \{0, \ldots, n\} \right\} \) for \( n \geq 2 \) that contains the tetrahedra

\[
T_{i,j,k} := \text{conv} \left\{ \left( \frac{i}{n}, \frac{j}{n}, \frac{k}{n} \right), \left( \frac{i+1}{n}, \frac{j}{n}, \frac{k}{n} \right), \left( \frac{i}{n}, \frac{j+1}{n}, \frac{k}{n} \right), \left( \frac{i}{n}, \frac{j}{n}, \frac{k+1}{n} \right) \right\}
\]  
(5.14)

for each inner node \( \left( \frac{i}{n}, \frac{j}{n}, \frac{k}{n} \right) \in \mathcal{N}(B) \). We first define the Nédélec space

\[
\mathcal{N}_0^1(T; \mathbb{R}^{3\times 3}) = \{ \beta_h \in H_0(\text{Curl}; B; \mathbb{R}^{3\times 3}) : \beta_h = a + b \wedge x, a, b \in P_0(T; \mathbb{R}^{3\times 3}) \}
\]
and the Crouzeix-Raviart space

\[
\text{CR}^1(T; \mathbb{R}^3) = \{ a_h \in L^2(B; \mathbb{R}^3) : a_h|_T \in P_1(T; \mathbb{R}^3) \text{ for all } T \in \mathcal{T} \text{ and } a_h \text{ is continuous at the centroid of any face } F \in \mathcal{T}(B) \}.\]

**Lemma 3** Let \( d = 3 \) and \( \mathcal{T} \) be a simplicial regular triangulation. Let \( k \in \mathbb{N} \). There exists a \( \delta \lambda_h \in P_0(T; \mathbb{R}^{3\times 3}) \) such that

\[
0 = \sup_{(\delta u_h, \delta H_h) \in \mathcal{S}_0^1(T; \mathbb{R}^{3\times 3})} \frac{B((\delta u_h, \delta H_h), (\delta \lambda_h))}{\| \nabla \delta u_h \|_{L^2(B)} + \| \nabla \delta H_h \|_{L^2(B)}}.
\]  
(5.15)

**Proof.** Let \( \delta u_h \in S_0^1(T; \mathbb{R}^3) \) and \( \delta H_h \in S_0^1(T; \mathbb{R}^{3\times 3}) \) be arbitrary.

Consider the discrete Helmholtz decomposition\([32]\]

\[
P_0(T; \mathbb{R}^{3\times 3}) = \nabla_h \text{CR}^1(T; \mathbb{R}^3) \oplus \text{Curl} \mathcal{N}_0^1(T; \mathbb{R}^{3\times 3}).
\]  
(5.16)

We obtain with the \( L^2(B) \)-orthogonality of decomposition (5.16) for \( \delta \lambda_h = \text{Curl} \beta_h \) with \( \beta_h \in \mathcal{N}_0^1(T; \mathbb{R}^{3\times 3}) \) that

\[
B((\delta u_h, \delta H_h), (\delta \lambda_h)) = (\nabla \delta u_h, \text{Curl} \beta_h)_{L^2(B)} - (\delta H_h, \text{Curl} \beta_h)_{L^2(B)}
= - (\delta H_h, \text{Curl} \beta_h)_{L^2(B)}.
\]

Since the nullspace of \( \text{Curl} : \mathcal{N}_0^1(T; \mathbb{R}^{3\times 3}) \rightarrow P_0(T; \mathbb{R}^{3\times 3}) \) equals the range of \( \nabla : S_0^1(T; \mathbb{R}^3) \rightarrow \mathcal{N}_0^1(T; \mathbb{R}^{3\times 3}) \) (compare discrete exact sequences in Boffi et al.\([33]\)) it holds \( \text{dim} (\text{Curl}(\mathcal{N}_0^1(T; \mathbb{R}^{3\times 3}))) = 3(\# \mathcal{E}(B) - \# \mathcal{N}(B)) \).

We identify each inner node \( \left( \frac{i}{n}, \frac{j}{n}, \frac{k}{n} \right) \) with a tetrahedron \( T_{i,j,k} \) as defined in (5.14). For \( i, j, k \neq (i, j, k) \) it holds that the set of edges of the corresponding tetrahedra are disjoint, that is, \( \mathcal{E}(T_{i,j,k}) \cap \mathcal{E}(T_{i',j',k'}) = \emptyset \). Since \( \# \mathcal{E}(T_{i,j,k}) = 6 \) and \( \mathcal{E}(T_{i,j,k}) \) are inner edges for all inner nodes \( i, j, k \) it holds \( \# \mathcal{E}(B) \geq 6 \# \mathcal{N}(B) \). We thus obtain

\[
\text{dim}(S_0^1(T; \mathbb{R}^{3\times 3})) = 9 \# \mathcal{N}(B) < 3(\# \mathcal{E}(B) - \# \mathcal{N}(B)) = \text{dim}(\text{Curl}(\mathcal{N}_0^1(T; \mathbb{R}^{3\times 3}))).
\]

Thus, there exists a \( \beta_h \in \mathcal{N}_0^1(T; \mathbb{R}^{3\times 3}) \) with \( (\delta H_h, \text{Curl} \beta_h)_{L^2(B)} = 0 \) for all \( \delta H_h \in S_0^1(T; \mathbb{R}^{3\times 3}) \).

For further stability analysis of finite element spaces we will respectively use the following remark.

**Remark 1** Let \( d \in \mathbb{N} \). Let \( T \) be a quasi-uniform triangulation of \( B \) with mesh size \( \text{diam}(T) \approx h > 0 \) for all \( T \in \mathcal{T} \).

Given an inner node \( k \) of \( T \). Let \( \delta \lambda_k := \phi_k \) be the corresponding hat function, that is, it is piecewise affine and satisfies \( \phi_k(j) = \delta_{jk} \) for every node \( j \) and for the Kronecker delta \( \delta_{jk} \). A Poincaré inequality on the nodal patch proves that \( \| \delta \lambda_k \|_{L^2(B)} \leq c h \| \nabla \delta \lambda_k \|_{L^2(B)} \) for a constant \( c > 0 \).

**Remark 2** Let \( d = 2, 3 \). Consider the conforming discretization with \( \delta \lambda_h \in S_0^1(T; \mathbb{R}^{d \times d}), \delta H_h \in S_0^1(T; \mathbb{R}^{d \times d}) \) and \( \delta u_h \in S_0^1(T; \mathbb{R}^d) \). The choices \( \delta u_h = 0 \) and \( \delta H_h = -\delta \lambda_h \) yield an inverse inequality for a constant \( c > 0 \)

\[
\sup_{\delta u_h \in S_0^1(T; \mathbb{R}^d), \delta H_h \in S_0^1(T; \mathbb{R}^{d \times d})} \frac{B((\delta u_h, \delta H_h), (\delta \lambda_h))}{\| \nabla \delta u_h \|_{L^2(B)} + \| \nabla \delta H_h \|_{L^2(B)}}
\]
\[ \geq \| \delta \lambda_h \|_{L^2(B)}^2 \geq c h^2 \| \nabla \delta \lambda_h \|_{L^2(B)}^2 \geq c h^2 \| \nabla \delta \lambda_h \|_{L^2(B)}. \]

On the other hand, Remark 1 shows that there is a \( \delta \lambda_h \in S_0^1(T ; \mathbb{R}^{d \times d}) \) such that

\[ \sup_{\delta u_h \in S_0^1(T ; \mathbb{R}^2), \delta H \in S_0^1(T ; \mathbb{R}^{d \times d})} \frac{B((\delta u_h, \delta H), \delta \lambda_h)}{\| \nabla \delta u_h \|_{L^2(B)} + \| \nabla \delta H \|_{L^2(B)}} \leq h \| \nabla \delta \lambda_h \|_{L^2(B)}. \]

Thus, there exists a discrete solution but the stability depends on \( h \).

### 5.2.2 Existence of a discrete solution and influence of the domain size

This section proves stability of a P2-P1B-P0 discretization (P1B denoting the space of P1 functions enriched by volume bubbles) for \( d = 2 \) under a condition on the size of \( B \). The stability is proven with respect to a nonstandard mesh-dependent norm of \( \lambda \). This implies that a unique discrete solution exists. Note that convergence of the discrete solution does not follow from Brezzi’s splitting theorem due to the missing stability of the continuous problem (3.7).

Recall the definition of the Crouzeix-Raviart space \( \text{CR}^1(T ; \mathbb{R}^2) \) from Lemma 2 and define

\[ \text{CR}_0^1 := \{ u_{\text{CR}} \in \text{CR}^1 : u_{\text{CR}}(p) = 0 \text{ for all midpoints } p \text{ of boundary edges } e \in \mathcal{E}(\partial B) \}. \]

Lemma 4 is used in Proposition 2.

**Lemma 4** There exists a constant \( C < \infty \) such that

\[ \| \nabla_h \delta u_{\text{CR}} \|_{L^2(B)} \leq C \sup_{\delta u_h \in \text{CR}_0^1(T ; \mathbb{R})} \frac{\| \nabla \delta u_h \|_{L^2(B)}}{\| \nabla \delta u_h \|_{L^2(B)}} \]

for all \( \delta u_{\text{CR}} \in \text{CR}_0^1(T ; \mathbb{R}^2) \). Here \( \nabla_h \) denotes the \( T \)-piecewise gradient.

**Proof.** Given \( \delta u_{\text{CR}} \in \text{CR}_0^1(T) \), let \( \delta u_h := J_2 \delta u_{\text{CR}} \) with the companion operator \( J_2 : \text{CR}_0^1(T ; \mathbb{R}^2) \to S_0^1(T ; \mathbb{R}^2) \) from Carstensen and Schedensack.\(^{[34, \text{Lemma 3.3}]} \) This operator has the property that the \( \| \nabla \cdot \delta u_{\text{CR}} \|_{L^2(B)} \) equals \( \nabla_h \delta u_{\text{CR}} \). This and the stability of \( J_2 \) prove \( \| \nabla \delta u_h \|_{L^2(B)} = \| \nabla \delta u_{\text{CR}} \|_{L^2(B)} \) and \( \| \nabla \delta u_h \|_{L^2(B)} \leq C \| \nabla_h \delta u_{\text{CR}} \|_{L^2(B)} \).

Let \( C_{\text{inf sup, Curl}} \) denote the constant from the inf-sup condition for the mini-FEM\(^{[30]} \)

\[ C_{\text{inf sup, Curl}} \| \beta_h \|_{L^2(B)} \leq \sup_{\delta H \in S_0^1(T ; \mathbb{R}^{2 \times 2}) \oplus (\text{Cur}(S^1(T ; \mathbb{R}^2) \cap L^2_0(B ; \mathbb{R}^2)))} \frac{(\delta H \cdot \text{Curl} \beta_h)}{\| \nabla \delta H \|_{L^2(B)}} \] (5.17)

for all \( \beta_h \in S_0^1(T ; \mathbb{R}^2) \cap L^2_0(B ; \mathbb{R}^2) \). Let \( \delta \lambda_h \in P_0(T ; \mathbb{R}^{2 \times 2}) \). The discrete Helmholtz decomposition for \( d = 2 \) \( P_0(T ; \mathbb{R}^{2 \times 2}) = \nabla_h \text{CR}_0^1(T ; \mathbb{R}^2) \oplus \text{Cur}(S^1(T ; \mathbb{R}^2) \cap L^2_0(B ; \mathbb{R}^2)) \) with \( L^2_0(B ; \mathbb{R}^2) := \{ v \in L^2_0(B ; \mathbb{R}^2) : \int_B vdx = 0 \} \) guarantees the existence of \( \alpha_{\text{CR}} \in \text{CR}_0^1(T ; \mathbb{R}^2) \) and \( \beta_h \in S^1(T) \cap L^2_0(B ; \mathbb{R}^2) \) with

\[ \delta \lambda_h = \nabla_h \alpha_{\text{CR}} + \text{Curl} \beta_h. \]

Define the discrete norm \( \| \cdot \|_h \) on \( P_0(T ; \mathbb{R}^{2 \times 2}) \) by

\[ \| \delta \lambda_h \|_h := \sqrt{\| \nabla_h \alpha_{\text{CR}} \|_{L^2(B)}^2 + \| \beta_h \|_{L^2(B)}^2}. \]

The following proposition guarantees the unique existence of a discrete solution for the discretization of (3.7) where the approximation of \( (u, H, \lambda) \) is sought in \( S^1_0(T ; \mathbb{R}^2) \times S^0_0(T ; \mathbb{R}^{2 \times 2}) \times P_0(T ; \mathbb{R}^{2 \times 2}) \), with \( S^1_0(T ; \mathbb{R}^{2 \times 2}) := S^1_0(T ; \mathbb{R}^{2 \times 2}) + \mathcal{B}(T ; \mathbb{R}^{2 \times 2}) \) and \( \mathcal{B}(T ; \mathbb{R}^{2 \times 2}) \) being the space of volume bubbles.
Furthermore, let $C_P$ denote the Poincaré constant, that is, the smallest constant such that $\|\beta\|_{L^2(B)} \leq C_P \|\nabla\beta\|_{L^2(B)}$ holds for all $\beta \in H^1_0(B; \mathbb{R}^2)$.

**Proposition 2** If $2C_{\text{infsup},\text{Curl}} - C_P > 0$, then there exists a $C > 0$ such that for all $\delta \lambda_h \in P_0(\mathcal{T}; \mathbb{R}^{2\times 2})$

\[
C\|\delta \lambda_h\|_h \leq \sup_{(\delta u_h, \delta H_h) \in S_0^0(\mathcal{T}; \mathbb{R}^{3\times 2}) + B(\mathcal{T}; \mathbb{R}^{2\times 2})} \frac{B((\delta u_h, \delta H_h), \delta \lambda_h)}{\|\nabla \delta u_h\|_{L^2(B)} + \|\nabla \delta H_h\|_{L^2(B)}}. \quad (5.18)
\]

**Proof.** Given $\delta \lambda_h = \nabla_h \alpha_{CR} + \text{Curl} \beta_h$ with $\alpha_{CR}$ and $\beta_h$ as above, set $\delta u_h := J_2 \alpha_{CR} \in S_0^0(\mathcal{T}; \mathbb{R}^2)$ with $J_2$ as in the proof of Lemma 4. This and the inf-sup condition of (5.17) guarantee the existence of $\delta H_h \in (S_0^0(\mathcal{T}; \mathbb{R}^{2\times 2}) + B(\mathcal{T}; \mathbb{R}^{2\times 2}))$ with $\|\nabla \delta H_h\|_{L^2(B)} = \|\beta_h\|_{L^2(B)}$ and

\[
(1/2) C_{\text{infsup},\text{Curl}} \|\beta_h\|_{L^2(B)}^2 \leq (\delta H_h, \text{Curl} \beta_h)_{L^2(B)}.
\]

Then,

\[
B((\delta u_h, \delta H_h), \delta \lambda_h) \geq \|\nabla_h \alpha_{CR}\|_{L^2(B)}^2 + (\delta H_h, \nabla_h \alpha_{CR})_{L^2(B)} + (\delta H_h, \text{Curl} \beta_h)_{L^2(B)}
\]

\[
\geq \|\nabla_h \alpha_{CR}\|_{L^2(B)}^2 + (1/2) C_{\text{infsup},\text{Curl}} \|\beta_h\|_{L^2(B)}^2 - \|\delta H_h\| \|\nabla_h \alpha_{CR}\|_{L^2(B)}.
\]

The Poincaré inequality and a weighted Young inequality lead for any $\epsilon > 0$ to

\[
\|\delta H_h\|_{L^2(B)} \|\nabla_h \alpha_{CR}\|_{L^2(B)} \leq (\epsilon/2) \|\nabla_h \alpha_{CR}\|_{L^2(B)}^2 + (C_P/(2\epsilon)) \|\beta_h\|_{L^2(B)}^2.
\]

The combination of the above inequalities proves

\[
B((\delta u_h, \delta H_h), \delta \lambda_h) \geq (1 - (\epsilon/2)) \|\nabla_h \alpha_{CR}\|_{L^2(B)}^2 + (1/2) C_{\text{infsup},\text{Curl}} - C_P/(2\epsilon) \|\beta_h\|_{L^2(B)}^2
\]

\[
\geq \min \left\{1 - \frac{\epsilon}{2}, \frac{C_{\text{infsup},\text{Curl}}}{2} - \frac{C_P}{2\epsilon}\right\} \|\delta \lambda_h\|_h^2.
\]

For $\epsilon = 1 + C_P/(2C_{\text{infsup},\text{Curl}})$ the minimum is positive. This together with $\|\nabla_h \alpha_{CR}\|_{L^2(B)} + \|\beta_h\|_{L^2(B)}^2 = \|\delta \lambda_h\|_h^2$ proves (5.18). \hfill \Box

**Remark 3** While $C_{\text{infsup},\text{Curl}}$ does only depend on the shape of $B$, the Poincaré constant $C_P$ depends on the diameter of $B$. Therefore, the inequality $2C_{\text{infsup},\text{Curl}} - C_P > 0$ is satisfied if the diameter of $B$ is sufficiently small.

**Lemma 5** Let $\mathcal{T}$ be a quasi-uniform triangulation. There exists a constant $C > 0$ such that

\[
h \|\delta \lambda_h\| \leq C \|\delta \lambda_h\|_h \quad \text{for all} \quad \delta \lambda_h \in P_0(\mathcal{T}; \mathbb{R}^{2\times 2}). \quad (5.19)
\]

**Proof.** An inverse estimate proves that there exists a constant $C > 0$ such that for any $\beta_h \in S_0^1(\mathcal{T}; \mathbb{R}^2) \cap L_0^2(B; \mathbb{R}^2)$

\[
h \|\text{Curl} \beta_h\| \leq C \|\beta_h\|.
\]

Therefore, for $\delta \lambda_h \in P_0(\mathcal{T}; \mathbb{R}^{2\times 2})$ with $\delta \lambda_h = \nabla_h \alpha_{CR} + \text{Curl} \beta_h$ with $\alpha_{CR} \in CR_0^1(\mathcal{T}; \mathbb{R}^2)$ and $\beta_h \in S^1(\mathcal{T}; \mathbb{R}^2) \cap L_0^2(B; \mathbb{R}^2)$ it follows

\[
\|\delta \lambda_h\|^2 \leq (\|\nabla_h \alpha_{CR}\| + \|\text{Curl} \beta_h\|)^2 \leq 2\|\nabla_h \alpha_{CR}\|^2 + 2C^2 h^{-2} \|\beta_h\|^2 \leq 2C^2 h^{-2} \|\delta \lambda_h\|^2. \quad \Box
\]

The inequality (5.19) is in fact sharp: For $\delta \lambda_h = \text{Curl} \phi_h$ with $\phi_h$ a hat function in $S_0^1(\mathcal{T})$ we conclude with Remark 1 that there exists a constant $c > 0$ with

\[
h \|\delta \lambda_h\|_{L^2(B)} = h \|\text{Curl} \phi_h\|_{L^2(B)} = h \|\nabla \phi_h\|_{L^2(B)} \geq c \|\phi_h\|_{L^2(B)} = c \|\text{Curl} \phi_h\|_h = c \|\delta \lambda_h\|_h.
\]
Further finite elements, which are part of the numerical investigation are presented in Table 2. The notation $Q_k(B;\mathbb{R}^d)$ is introduced for polynomials corresponding to $k$th order Lagrange quadrilaterals for $d = 2$ and hexahedrals for $d = 3$.

### 6 | NUMERICAL EXAMPLES

In this section the proposed discretizations are numerically evaluated with regard to the finite element convergence as well as to stability. In order to keep the focus on the finite element discretization a comparatively simple material model is considered. The gradient enriched strain energy density consists of an additively decomposed local and nonlocal part

$$W(F, \nabla F) = W^{\text{loc}}(F) + W^{\text{nloc}}(\nabla F).$$

Here, we choose a classical compressible Neo-Hooke energy for $W^{\text{loc}}(F)$ and thus,

$$W^{\text{loc}}(F) = \frac{\lambda}{2}(I_1^{1/2} - 1)^2 - \mu \ln I_3^{1/2} + \frac{\mu}{2}(I_1 - 3).$$

Herein, the invariants $I_1 = \text{tr} C$ and $I_3 = \det C$ are functions of the right Cauchy Green tensor. For the Lamé parameters $\lambda(E, \nu), \mu(E, \nu)$ the elastic constants $E = 250$ MPa and $\nu = 0.3$ have been chosen. The gradient enriched part of the strain energy is chosen as

$$W^{\text{nloc}}(\nabla F) = \frac{\kappa}{2} \nabla F \cdot \nabla F,$$

which is quadratic in $\nabla F$. The frame indifference and isotropy of $W^{\text{nloc}}$ was proven in Triantafyllidis and Aifantis.\cite{22}\ The constitutive parameter $\kappa \geq 0$ of the gradient enrichment can be linked to a microstructural length-parameter with $l = \sqrt{\kappa/\mu}$.\cite{3,21}\ For the following numerical examples the nonlocal length-parameter is set to $l = 0.1$ mm.

#### 6.1 | Unit square test

In order to analyze the convergence behavior for the case $d = 2$, a unit square domain $B$ with the dimensions $1 \times 1$ mm$^2$ (cf. Figure 1A) is considered. The constitutive model is implemented under the plain strain assumption. For the construction of an error estimator the displacement field is predefined as reference solution by

$$u(X) = [0, \beta b(X)^2]^T, \text{ with } b(X) = XY(X - 1)(Y - 1)\quad (6.4)$$

where $\beta = -50$ mm$^{-8}$ is a scaling factor so that the order of magnitude of the displacement $(u(0.5, 0.5) = -0.1953$ mm) is within the nonlinear elastic range. Furthermore, the displacement field has the property $u|_{\partial B} = 0$ and $\nabla u|_{\partial B} = 0$. Consequently, the resulting body forces $f$ of the gradient elasticity problem can be analytically computed with the strong form

$$\text{Div} P - \text{Div}(\text{Div} G) = -f \text{ with } u|_{\partial B} = 0 \text{ and } \nabla u|_{\partial B} = 0,$$\quad (6.5)
which is obtained by variation of (2.5). By imposing \( f \) as external loading to the discrete boundary value problem (5.9), the finite element solution is compared to the P2 interpolation of the reference solution in the relative L 2-norm, that is, 
\[
\eta = \frac{\|I_2(u) - u_h\|_{L^2(B)}}{\|I_2(u)\|_{L^2(B)}},
\]
with P2 interpolation \( I_2(u) \) of the exact solution. It can be seen from Figure 1B that for uniform mesh refinement convergence order of \( h^2 \) is reached for the elements P2-P1B-P0 and P2-P1B-P1, whereas the order \( h^3 \) is obtained by the element P2-P2-P1, with \( h \) being the element diameter. Since the P2 interpolation \( I_2(u) \) converges with order \( h^3 \) to the exact solution, the convergence rates of the discrete solutions to the exact solution is \( h^2 \) for the elements P2-P1B-P0 and P2-P1B-P1 and \( h^3 \) for the element P2-P2-P1. Furthermore, the same convergence rates are obtained when measuring the error in the relative H1-seminorm \( \theta = \|I_2(u) - H_h\|_{L^2(B)}\|I_2(u)\|_{L^2(B)} \). However, the element P2-P1B-P0 has evoked an interruption of the linear solver at the refinement stage corresponding to \( h = 0.011 \) mm such that the last possible solution was obtained for this observation in correspondence to Remark 3, stating that the stability of this element depends on the size of the computational domain \( B \). The fact, that this additional stability issue is uncovered already on this simple unit cube domain makes the P2-P1B-P0 element an unsuitable choice of discretization. To analyze this further, Figure 1C unveils an \( h^2 \)-degeneration of minimal singular values of the submatrix \( K^T_B = [K^T_{uA}, K^T_{H_h}] \). This corresponds to the considerations in Section 5.2 and may ultimately lead to a loss of invertibility of the global tangent matrix due to close to zero minimal singular values. For the performed refinement stages, yet, this has not occurred for elements Q2-Q2-Q1, P2-P1B-P1, and P2-P2-P1. Note that the results for elements P2-P1-P0 and Q2-Q1-P0 are not depicted because zero minimal singular values of the global tangent matrix \( K \) occurred at all refinement stages precluding the solution of the linearized system of equations.
To investigate the three dimensional elements corresponding to the considered approximations, the unit square problem of Section 6.1 is adapted to a three-dimensional unit cube with the dimensions $1 \times 1 \times 1$ mm$^3$. Consequently, the displacement field (6.4) is adjusted with

$$u(X) = \left[ 0, 0, \beta b(X)^2 \right]^T, \quad \text{with} \quad b(X) = XYZ(X-1)(Y-1)(Z-1)$$

and $\beta = -1000$ mm$^{-18}$ leading to a maximal reference displacement of $u(0.5, 0.5, 0.5) = -0.2441$ mm. Convergence characteristics (cf. Figure 2B) of all investigated discretizations are in accordance to the two-dimensional case. Similar to Section 6.1, the element P2-P1B-P0 evokes an interruption of the linear solver at a mesh refinement stage corresponding to $h = 0.108$ mm, which may again be in correspondence to Remark 3. While the minimal singular values of the tangent matrix of all elements degenerate as in the 2D-case, a loss of invertibility of the global linearized system of equations corresponding to the P2-P1B-P1, P2-P2-P1, and Q2-Q2-Q1 discretization has again not been observed. It is notable, that the tangent matrix of the element Q2-Q1-P0, which is singular at all refinement stages, can be numerically stabilized by superposing it with a diagonal matrix $\gamma I$ of the same dimension, with $\gamma \in \mathbb{R}^{>0}$ and $\gamma \ll 1$. This may however induce an error, since the discrete system does not correspond to the initial formulation anymore. In Figure 2A, the relative displacement $\nu = u_Z^e(X)/u_Z(X)$ at the center point $X = (0.5, 0.5, 0.5)^T$ is plotted over the total computing time needed for the solution procedure. Summarizing, the elements Q2-Q2-Q1 and P2-P2-P1 have a favorable convergence behavior in this particular boundary value problem.

### 6.3 3D Cook’s problem

In the 3D Cook’s problem (Figure 3A) the body is clamped on one side and loaded with surface traction on the other side. Thus, the assumption of essential boundary conditions applied to the whole boundary, made at the end of Section 3, is modified to $u |_{\Gamma_D} = 0$ and $\Gamma_N = \emptyset$ with a surface traction $f = (0, 0, 6.25 \text{ MPa})^T$. In order to compare the convergence behavior of the elements, in Figure 3B the relative displacement in Z-direction, measured at the corner point $A = (48, 20, 60)$ mm, is plotted over the number of degrees of freedom. Since an analytical reference solution is not available for this problem, the reference displacement $u_Z = 8.76$ mm depicts the numerical solution at a high mesh refinement stage, in which the solutions of all considered elements are in concordance within an accuracy of three significant figures. In order to show the ability to avoid mesh dependent solutions due to singularities the nonlocal formulation using a P2-P2-P1 element is compared to a classical local formulation using a quadratic tetrahedral, that is, $P2:= \{ Vh = S^2(T; \mathbb{R}^3) \}$. The latter formulation is obtained if the terms...
### TABLE 3  
Stability characteristics of the investigated elements (subscripts indicate that the finding is restricted to the 2D or 3D case)

| Element name   | Mathematical analysis | Numerical results 2D | Numerical results 3D |
|----------------|------------------------|----------------------|----------------------|
| P1-P1-P0       | 1<sub>2D</sub>         | 1                    | 1                    |
| P2-P1-P0       | 1<sub>3D</sub>         | 2,3                  | 2,3                  |
| P2-P1B-P0      | 2<sub>2D</sub>, 3<sub>2D</sub> | 2                    | 2                    |
| P2-P1B-P1      |                        | 2                    | 2                    |
| P2-P2-P1       |                        | 2                    | 2                    |
| Q2-Q1-P0       | 1                      | 1                    | 1                    |
| Q2-Q2-Q1       | 2                      | 2                    | 2                    |

**Legend**

|   |   |   |   |
|---|---|---|---|
| 1 | Not stable | Singular tangent | Singular tangent |
| 2 | Stability depends on $h$ | $\sigma_{\text{min}}(K_B) \propto h^2$ | $\sigma_{\text{min}}(K_B) \propto h^3$ |
| 3 | Stability depends on $B$ | Lin. solv. interrupt | Lin. solv. interrupt |

in (5.2) containing the additional field variables are neglected, yielding

$$\Pi^h_e = \int_{B_e} W(F(u^h_e)) \, dV + \Pi^h_{e,\text{ext}}(u^h_e).$$

(6.7)

In Figure 3D the absolute values of $F_{YX}$ at the strain concentration point $B = (0, 0.44)^T$ are plotted over the element size according to the mesh refinement stage. In order to obtain comparability $F_{YX}$ is evaluated as postprocessing quantity of $u^h$ for both elements despite the fact that for element P2-P2-P1 $F_{YX}$ could be directly evaluated from $H^h$. It becomes evident that as $h$ decreases, the $F_{YX}$-values of the P2-element diverge to infinite absolute values, while those of the P2-P2-P1 element are bounded. This illustrates one of the advantages of the gradient elasticity approach over classical formulations also at finite strains.

### 7  CONCLUSION

The three-field mixed formulation for gradient elasticity (cf. Shu et al.[27, 28] for the small strain framework) was generalized to the finite strain hyperelastic setting. Mathematical analysis in the linear framework of the continuous formulation has unveiled instability with respect to the standard norms and Brezzi’s splitting lemma. Moreover, for the finite element space P1-P1-P0 in 2D and P2-P1-P0 in 3D the discrete inf-sup condition does not hold. Although instability of the linear formulation most likely implies instability of nonlinear formulations, the mathematical stability analysis is still missing and open problem for future research. However, three-field formulations similar to the ones investigated here have been proposed in the literature not only in the context of gradient elasticity at small strains.[27, 28] Also for gradient damage at large strains similar mixed formulations have been proposed,[35, 36] where any mathematical analysis (also of the continuous problem) is still missing. Therefore, a comprehensive numerical study on all elements has been conducted at finite strains in order to show potential problems resulting from the expected instabilities at large strains, which were indeed numerically verified. Interestingly, numerical experiments have however also shown that for some finite strain elements (e.g., P2-P2-P1 and Q2-Q2-Q1) discrete instabilities have not occurred and finite element convergence could be observed. In addition, the numerically converged solutions of Section 6.1 and 6.2 are in concordance with the exact analytical solution. Also, the displacement convergence plot of the 3D Cook’s problem of Section 6.3 unveils concurrent numerically converged solutions of the elements Q2-Q2-Q1, P2-P2-P1, P2-P1B-P1 and P2-P1B-P0. In summary, numerical convergence to different solutions could not be observed. This is mostly due to the fact, that although their quadratic order of decreasing minimal singular values with decreasing element size is unsatisfying (cf. Figure 1C), still suitable numerical results may be obtained as long as the minimal singular values do not approach zero before finite element convergence is reached. An overview of the observations regarding the investigated elements is given in Table 3. However, the fact that individual calculations converging to the solution were obtained even for the potentially unstable formulations should not be mistaken as indicator for a suitable FE formulation, since it is in general unclear if the converged solution is the solution to the problem. A mesh-sensitivity test on the 3D Cook’s problem has shown the advantage of the gradient elasticity approach over a classical elasticity element even at finite strains. This motivates further research on robust and efficient finite element schemes, which avoid the observed instability issues.
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APPENDIX A

Define the following matrix dimensions as

\[ d \in \{2, 3\}, \quad u = \dim d_u^e, \quad h = \dim d_H^e, \quad \text{and} \quad s = \dim d_s^e. \]  
(A.1)

A suitable matrix notation for the derivatives is given by

\[ \nabla u^h = B_u^e d_u^e \quad \text{and} \quad \nabla H^h = B_H^e d_H^e. \]  
(A.2)

wherein \( B_u^e \in \mathbb{R}^{d_u^e \times u} \) and \( B_H^e \in \mathbb{R}^{d_H^e \times h} \) are appropriate B-matrices including the first order derivatives of the shape functions belonging to \( N_u^e \) and \( N_H^e \). Using these matrices, the analogous expressions for the variations and increments of the degrees of freedom are obtained. Let \( P, G, C_{\text{loc}}, \) and \( C_{\text{nloc}} \) denote analogous matrix notations for

\[ \frac{\partial W(d_u^e)}{\partial F}, \quad \frac{\partial W(d_H^e)}{\partial F}, \quad \frac{\partial^2 W(d_u^e)}{\partial F^2}, \quad \text{and} \quad \frac{\partial^2 W(d_H^e)}{\partial F^2}. \]  
(A.3)

Then the differentiation of the discrete potential (5.1) with respect to the element degrees of freedom yields the element residual vectors

\[ r_u^e = \frac{\partial \Pi_h^e}{\partial d_u^e} = \int_{B_e} \left( (B_u^e)^T P - (B_u^e)^T \lambda \right) dV + r_{\text{ext}}^e \quad \in \mathbb{R}^u \]  
(A.4)

\[ r_H^e = \frac{\partial \Pi_h^e}{\partial d_H^e} = \int_{B_e} \left( (B_H^e)^T G + (N_H^e)^T \lambda \right) dV \quad \in \mathbb{R}^h \]  
(A.5)

\[ r_s^e = \frac{\partial \Pi_h^e}{\partial d_s^e} = \int_{B_e} (N_s^e)^T (H - \nabla u) dV \quad \in \mathbb{R}^s \]  
(A.6)

By further differentiation of (5.6) with respect to the element degrees of freedom the components of the element tangential matrix is obtained as

\[ k_{uu}^e = \frac{\partial r_u^e}{\partial d_u^e} = \int_{B_e} (B_u^e)^T C_{\text{nloc}} B_u^e \quad \in \mathbb{R}^{u \times u} \]  
(A.7)

\[ k_{uH}^e = \frac{\partial r_u^e}{\partial d_H^e} = 0 \quad \in \mathbb{R}^{u \times h} \]  
(A.8)

\[ k_{u\lambda}^e = \frac{\partial r_u^e}{\partial d_s^e} = -\int_{B_e} (B_u^e)^T N_s^e \quad \in \mathbb{R}^{u \times s} \]  
(A.9)

\[ k_{Hu}^e = \frac{\partial r_H^e}{\partial d_u^e} = 0 \quad \in \mathbb{R}^{h \times u} \]  
(A.10)

\[ k_{HH}^e = \frac{\partial r_H^e}{\partial d_H^e} = \int_{B_e} (B_H^e)^T C_{\text{nloc}} B_H^e \quad \in \mathbb{R}^{h \times h} \]  
(A.11)

\[ k_{H\lambda}^e = \frac{\partial r_H^e}{\partial d_s^e} = \int_{B_e} (N_H^e)^T N_s^e \quad \in \mathbb{R}^{h \times s} \]  
(A.12)

\[ k_{u\lambda}^e = \frac{\partial r_s^e}{\partial d_u^e} = -\int_{B_e} (N_s^e)^T B_u^e \quad \in \mathbb{R}^{s \times u} \]  
(A.13)

\[ k_{H\lambda}^e = \frac{\partial r_s^e}{\partial d_H^e} = \int_{B_e} (N_s^e)^T N_H^e \quad \in \mathbb{R}^{s \times h} \]  
(A.14)

\[ k_{s\lambda}^e = \frac{\partial r_s^e}{\partial d_s^e} = 0 \quad \in \mathbb{R}^{s \times s} \]  
(A.15)

It becomes evident that the element tangent matrix is symmetrical.