Linear-programming approach to nonconvex variational problems

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Abstract. In nonconvex optimization problems, in particular in nonconvex variational problems, there usually does not exist any classical solution but only generalized solutions which involve Young measures. In this paper, after reviewing briefly the relaxation theory for such problems, an iterative scheme leading to a "sequential linear programming" (=SLP) scheme is introduced, and its convergence is proved by a Banach fixed-point technique. Then an approximation scheme is proposed and analyzed, and calculations of an illustrative 2D "broken-extremal" example are presented.

Key Words. Young measures, convex approximations, relaxed variational problems, linear approximation, Banach fixed point, adaptive scheme.

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1. Introduction

Nonconvex optimization problems often lack any solution because of fast oscillations of minimizing sequences that eventually break lower semicontinuity with respect to a weak convergence, cf. [44] and references therein for a survey in case of scalar variational problems on which we will focus in this paper. Therefore, a relaxation is urgent to solve such problems in a suitably generalized sense. The most general way of relaxation is certainly a suitable continuous extension, using also a suitable linear-space structure not necessarily completely coherent with the linear structure occuring in the formulation of the original problem. Thus extended, also called *relaxed*, problems then may get a convex structure even if the original problem does not have any. For a large class of problems, (generalized) *Young measures* (cf. e.g. [2, 42]) represent a suitable tool.

The relaxed problems can be discretized by a theory of approximation of (generalized) Young measures developed recently in [40, 41, 42], see also [32, 37, 38]. Numerical solution of the relaxed problems can be often performed directly, without approximating the original, non-relaxed problem, cf. [27, 28, 29, 32, 33, 34, 35, 42, 43]. If the (additively coupled, cf. e.g. ($\mathfrak{P}$) below) problem is linear in a lower-order term (i.e. $G(x,\cdot)$ in ($\mathfrak{P}$) is linear), such approach leads to a linear-programming problem and was shown very efficient in [4]. In the quadratic case, it naturally leads to a quadratic-programming problem, which is a considerably less efficient but still possible approach if the dimensionality is not too high, cf. [13, 32, 29, 43]. For non-quadratic case, one can still consider an iterative scheme leading to sequential-quadratic-programming algorithm, which is however even less efficient, cf. [31]. For other numerical approaches for the approximation of nonconvex variational problems we refer to [8, 11, 12, 14, 16, 17, 30].

Therefore, especially in a multidimensional case, a more efficient approach is desirable. We propose to approximate the relaxed problem not quadratically (in contrast to [31]) but linearly so that the auxiliary problems are as those in [4]. The idea of so-called *sequential linear programming* (=SLP) is not completely new and has been used in other context, e.g., in [19, 36, 49].

The goal of this paper is to demonstrate the usage of this, otherwise fairly (though not absolutely) general approach, on a concrete problem of scalar multidimensional variational calculus:

$$(\mathfrak{P}) \qquad \left\{ \begin{array}{ll} \text{Minimize} & \Phi(u) := \displaystyle\int_\Omega F(x, \nabla u(x)) + G(x, u(x))\, \mathrm{d}x, \\ \text{subject to} & u \in W^{1,p}(\Omega), \quad u|_{\partial\Omega} = u_{\mathrm{D}}, \end{array} \right.$$

with $\Omega \subset \mathbb{R}^n$ a bounded domain with the Lipschitz boundary $\partial\Omega$ and $u_{\mathrm{D}} \in W^{1-1/p,p}(\partial\Omega)$ given. Let us point out that we confine ourselves to *additively coupled* problems, in contrast to general problems involving the functional $\Phi(u) := \int_\Omega \varphi(x, u(x), \nabla u(x))\mathrm{d}x$; i.e. we consider only the special case $\varphi(x, u, s) = F(x, s) + G(x, u)$. It should be mentioned that this restriction seems unfortunately quite important for the linearization and the Banach-fixed-point techniques because, e.g., the estimate (3.6) below does not seem to be transferable to the general case. For the case that G is affine in u the linearized problem equals $(\mathfrak{P})$ and we generalize existing error estimates for the approximation of relaxed formulations of $(\mathfrak{P})$ to nonquadratic growth conditions under general assumptions.

The outline and the main contributions of this paper read as follows: We introduce the employed relaxation of the nonconvex variational problem $(\mathfrak{P})$ in Section 2 and prove convergence of a linearization in Section 3. Section 4 is devoted to the numerical analysis of the linearized problems. Besides an a-priori error estimate that relates three different scales, we establish an a-posteriori estimate which allows for adaptive mesh refinement. An efficient and reliable iterative algorithm to solve the discrete problems is provided in Section 5. In Section 6 we report on the performance of our algorithm applied to a scalar 2-well problem which has been proposed in [8, 10] as a benchmark model problem for the numerical approximation of scalar nonconvex variational problems. Finally, Section 7 further illustrates (and outlines some widening of) applicability of our algorithm; in particular, modelling of compatible phase transitions in elastic solids, optimal shape design problems, and certain phase transitions in antiplane shear settings are mentioned there.

2. The Young-measure relaxation

In this section we define the employed relaxation of $(\mathfrak{P})$ which is a continuous extension of $(\mathfrak{P})$ to measure valued solutions and has been established, e.g., in [42]. We briefly state the relaxed problem $(\mathfrak{RP})$ and the main results concerning the connections between $(\mathfrak{P})$ and $(\mathfrak{RP})$.

Let $M_1^+(\mathbb{R}^n)$ be the set of probability measures on $\mathbb{R}^n$, i.e., the set of all non-negative Radon measures μ satisfying $\int_{\mathbb{R}^n} \mu(\mathrm{d}s) = 1$. The set of L^p-*Young measures*

$\mathcal{Y}^p(\Omega;\mathbb{R}^n)$ is defined as

$$(2.1)\quad \mathcal{Y}^p(\Omega;\mathbb{R}^n):=\Big\{\nu\in L^\infty_{\mathrm{w}}(\Omega;M_1^+(\mathbb{R}^n)):\int_\Omega\int_{\mathbb{R}^n}|s|^p\nu_x(\mathrm{d}s)\,\mathrm{d}x<\infty\Big\}.$$

Here $\nu_x:=\nu(x)\in M_1^+(\mathbb{R}^n)$ for almost all $x\in\Omega$ and the index "w" in $L^\infty_{\mathrm{w}}(\Omega;M_1^+(\mathbb{R}^n))$ stands for "weakly* measurable", which means that given any $v\in C_0(\mathbb{R}^n):=\{w\in C(\mathbb{R}^n):\lim_{|s|\to\infty}w(s)=0\}$ the mapping $x\mapsto\int_{\mathbb{R}^n}v(s)\nu_x(\mathrm{d}s)$ is Lebesgue measurable in Ω.

The fundamental theorem on Young measures [2] (cf. also [42, Lemma 3.2.7]) allows to compute weak limits of continuous functionals applied to weakly convergent sequences in L^p. We will assume that $F:\Omega\times\mathbb{R}^n\to\mathbb{R}$ and $G:\Omega\times\mathbb{R}\to\mathbb{R}$ are Carathéodory functions satisfying, for almost all $x\in\Omega$, all $s\in\mathbb{R}^n$, and all $u\in\mathbb{R}$,

$$(2.2)\qquad c_1|s|^p\le F(x,s)\le c_2(1+|s|^p),$$

$$(2.3)\qquad |G(x,u)|\le a(x)+c_3|u|^q,$$

where $p>1$, $c_1,c_2,c_3>0$, $a\in L^1(\Omega)$, and $1<q<pn/(n-p)$ if $p<n$ and $1<q<\infty$ if $p\ge n$. Then we will consider the already annonced relaxed problem in the form:

$$(\mathfrak{RP})\qquad\left\{\begin{array}{ll}\text{Minimize} & \bar\Phi(u,\nu):=\displaystyle\int_\Omega\Big[\int_{\mathbb{R}^n}F(x,s)\nu_x(\mathrm{d}s)+G(x,u(x))\Big]\,\mathrm{d}x,\\ \text{subject to} & \displaystyle\int_{\mathbb{R}^n}s\nu_x(\mathrm{d}s)=\nabla u(x)\quad\text{for a.a. } x\in\Omega,\\ & u\in W^{1,p}(\Omega),\quad \nu\in\mathcal{Y}^p(\Omega;\mathbb{R}^n),\quad u|_{\partial\Omega}=u_{\mathrm{D}}.\end{array}\right.$$

The following assertion [13], showing that $(\mathfrak{RP})$ is indeed a proper relaxation of $(\mathfrak{P})$, is based on results from [25] and, in fact, translates some results of [42, Propositions 5.2.1, 5.2.6 and 3.4.15]:

Proposition 2.1. (See [13, Proposition 1]) *Assume (2.2) and (2.3). There holds:*
(i) $(\mathfrak{RP})$ *admits a solution.*
(ii) $\inf(\mathfrak{P})=\min(\mathfrak{RP})$.
(iii) *The embedding* $\iota: W^{1,p}(\Omega)\to W^{1,p}(\Omega)\times\mathcal{Y}^p(\Omega;\mathbb{R}^n)$, $v\mapsto(v,\delta_{\nabla v})$, *of any infimizing sequence for* $(\mathfrak{P})$ *has a weakly convergent subsequence whose (weak×weak*) limit is a solution to* $(\mathfrak{RP})$.
(iv) *Each solution to* $(\mathfrak{RP})$ *is the (weak × weak*) limit of the embedding* $\iota: W^{1,p}(\Omega)\to W^{1,p}(\Omega)\times\mathcal{Y}^p(\Omega;\mathbb{R}^n)$ *of some infimizing sequence for* $(\mathfrak{P})$.

3. An iterative algorithm to approximate $(\mathfrak{RP})$

The relaxation obviously linearized the problem as far as the highest term concerns. Also, the equality constraint in $(\mathfrak{RP})$ is linear. The only possibly nonlinear term in $(\mathfrak{RP})$ is $G(x,\cdot)$ and our iterative scheme will be based on a linearization of this term. This gives the following conceptual fixed-point algorithm $(\mathcal{A}_{\mathrm{FP}})$.

Algorithm $(\mathcal{A}_{\mathrm{FP}})$**.**

(a) Choose $\varepsilon_{\mathrm{FP}}>0$, $u^{(0)}\in W^{1,p}(\Omega)$, $u^{(0)}|_{\partial\Omega}=u_{\mathrm{D}}$, and set $k:=1$.

(b) Solve the following linear optimization problem ($(\mathfrak{RP}^{(k)})$):

$$(\mathfrak{RP}^{(k)})\qquad \begin{cases} \text{Minimize} & \bar{\Phi}^{(k)}(u,\nu) := \displaystyle\int_\Omega \Big[\int_{\mathbb{R}^n} F(x,s)\nu_x(\mathrm{d}s) \\ & \qquad\qquad + G'_u(x,u^{(k-1)})(u-u^{(k-1)}) \Big] \mathrm{d}x, \\ \text{subject to} & \displaystyle\int_{\mathbb{R}^n} s\nu_x(\mathrm{d}s) = \nabla u(x) \quad \text{for a.a. } x\in\Omega, \\ & u\in W^{1,p}(\Omega), \quad \nu\in\mathcal{Y}^p(\Omega;\mathbb{R}^n), \quad u|_{\partial\Omega}=u_{\mathrm{D}}. \end{cases}$$

Denote the solution to $(\mathfrak{RP}^{(k)})$ by $(u^{(k)},\nu^{(k)})$; assumptions made later will guarantee this solution to be unique.

(c) If $||u^{(k)}-u^{(k-1)}||_{L^2(\Omega)} \ge \varepsilon_{\mathrm{FP}}$, set $k := k+1$ and go to (b).

(d) Stop.

Throughout this article we assume, in addition to (2.2) and (2.3), that the convex hull of $F(x,\cdot)$, denoted by $F^{**}(x,\cdot)$, is continuously differentiable for almost all $x\in\Omega$ and there exist $c_4>0$, $\ell_G\ge 0$, and $s^*\in\mathbb{R}^n$, $|s^*|=1$, such that, for almost all $x\in\Omega$, for all all $s_1,s_2\in\mathbb{R}^n$, and all $u_1,u_2\in\mathbb{R}$, there holds

$$c_4(s^*\cdot(s_1-s_2))^2 \le \big([F^{**}]'_s(x,s_1)-[F^{**}]'_s(x,s_2)\big)\cdot(s_1-s_2), \tag{3.1}$$

$$|G'_u(x,u_1)-G'_u(x,u_2)| \le \ell_G|u_1-u_2|. \tag{3.2}$$

We must naturally assume $p\ge 2$ to make (2.2) and (3.1) mutually compatible. In order to exploit conventional weak-solution theory for the Euler-Lagrange equation related to $(\mathfrak{RP}^{(k)})$, we assume that there exist $c_5>0$ and $b\in L^{p'}(\Omega)$ such that, for almost all $x\in\Omega$ and for all $s\in\mathbb{R}^n$,

$$|[F^{**}]'_s(x,s)| \le b(x)+c_5(1+|s|^{p-1}). \tag{3.3}$$

Lemma 3.1. *Let* (3.1) *and* (3.3) *be valid. Then the mapping* $f\mapsto u : L^2(\Omega)\to L^2(\Omega)$, *with* $u\in W^{1,p}(\Omega)$ *solving in the weak sense the Dirichlet boundary value problem*

$$-\mathrm{div}\,\big([F^{**}]'_s(x,\nabla u)\big) = f, \qquad u|_{\partial\Omega}=u_{\mathrm{D}}, \tag{3.4}$$

is Lipschitz continuous with the constant ℓ_1 *given explicitly by*

$$\ell_1 = \frac{D_{\Omega,s^*}}{c_4}, \qquad D_{\Omega,s^*} := \mathrm{diam}\langle s^*,\Omega\rangle = \sup_{x_1,x_2\in\Omega} s^*\cdot(x_1-x_2). \tag{3.5}$$

Proof. Take two right-hand sides f_1 and f_2 and the corresponding weak solutions u_1 and u_2. Subtract the corresponding weak formulations from each other and test them by $u_1-u_2\in W^{1,p}_0(\Omega)$. By the fine version of Poincaré's inequality (which follows from the one-dimensional Poincaré inequality, see, e.g., Showalter [45, Ch.II, Lemma 5.1]) and by Hölder's inequality we get

$$\begin{aligned} \frac{1}{D_{\Omega,s^*}}||u_1-u_2||^2_{L^2(\Omega)} &\le \int_\Omega \big(s^*\cdot\nabla(u_1-u_2)\big)^2\mathrm{d}x \\ &\le \frac{1}{c_4}\int_\Omega \big([F^{**}]'_s(x,\nabla u_1)-[F^{**}]'_s(x,\nabla u_2)\big)\cdot\nabla(u_1-u_2)\mathrm{d}x \\ &= \frac{1}{c_4}\int_\Omega (f_1-f_2)(u_1-u_2)\mathrm{d}x \\ &\le \frac{1}{c_4}||f_1-f_2||_{L^2(\Omega)}||u_1-u_2||_{L^2(\Omega)}. \end{aligned} \tag{3.6}$$

□

For $\bar{u} \in W^{1,p}(\Omega)$, $\bar{u}|_{\partial\Omega} = u_{\rm D}$, let (u,ν) solve the following auxiliary problem:

$$(\mathfrak{AP}_{\bar{u}}) \quad \left\{ \begin{array}{ll} \text{Minimize} & \bar{\Phi}_{\bar{u}}(u,\nu) := \displaystyle\int_\Omega \left[\int_{\mathbb{R}^n} F(x,s)\nu_x(\mathrm{d}s) + G'_u(x,\bar{u})(u-\bar{u}) \right] \mathrm{d}x, \\ \text{subject to} & \displaystyle\int_{\mathbb{R}^n} s\nu_x(\mathrm{d}s) = \nabla u(x) \quad \text{for a.a. } x \in \Omega, \\ & u \in W^{1,p}(\Omega), \quad \nu \in \mathcal{Y}^p(\Omega;\mathbb{R}^n), \quad u|_{\partial\Omega} = u_{\rm D}. \end{array} \right.$$

The following Lemma 3.2 shows, in particular, uniqueness in terms of u-component of solutions to $(\mathfrak{AP}_{\bar{u}})$, which enables us to denote $u = S(\bar{u})$ for a solution (u,ν) to $(\mathfrak{AP}_{\bar{u}})$.

Lemma 3.2. *Let* (2.2), (2.3), *and* (3.1)–(3.3) *be valid. Then the mapping* $S : \bar{u} \mapsto u$, $L^2(\Omega) \to L^2(\Omega)$, *is Lipschitz continuous with the constant*

$$\ell_2 = \frac{D_{\Omega,s^*}\ell_G}{c_4}. \tag{3.7}$$

Proof. For (u,ν) solving $(\mathfrak{AP}_{\bar{u}})$, u must satisfy the Euler-Lagrange equation for the coarse relaxation of $(\mathfrak{AP}_{\bar{u}})$, i.e. for the problem of minimization of $\int_\Omega F^{**}(x,\nabla u) + G'_u(x,\bar{u})(u-\bar{u})\mathrm{d}x$ for $u \in W^{1,p}(\Omega)$, $u|_{\partial\Omega} = u_{\rm D}$. This equation is just (3.4) with $f = G'_u(x,\bar{u})$. Then, by (3.2), the mapping $\bar{u} \mapsto f : L^2(\Omega) \to L^2(\Omega)$ is obviously Lipschitz continuous with the constant ℓ_G. Composition of this mapping with the mapping $f \mapsto u$ addressed in Lemma 3.1 just gives the mapping S. Its Lipschitz constant ℓ_2 is $\ell_1\ell_G$, which is just (3.7). □

Lemma 3.3. *Let again* (2.2), (2.3), *and* (3.1)–(3.3) *be valid. Furthermore, let* $G(x,\cdot)$ *be "not much" nonconvex in the sense (formulated in terms of non-monotonicity of* G'_u*) that*

$$\begin{aligned} &\exists \gamma \geq -\frac{1}{\ell_1} \quad \forall u_1,u_2 \in \mathbb{R} \quad \forall (a.a.)\ x{\in}\Omega : \\ &\qquad \big(G'_u(x,u_1) - G'_u(x,u_2)\big)(u_1-u_2) \geq \gamma(u_1-u_2)^2, \end{aligned} \tag{3.8}$$

and let

$$D_{\Omega,s^*}\ell_G < c_4. \tag{3.9}$$

Then the mapping S *has a unique fixed point* u *and there is* ν *such that the pair* (u,ν) *solves the relaxed problem* $(\mathfrak{RP})$.

Proof. The fixed point $u \in W^{1,p}(\Omega) \subset L^2(\Omega)$ does exist by the Banach contraction-mapping principle. Yet, by the definition of S, $u = S(u)$ means that there is ν such that (u,ν) solves $(\mathfrak{RP}_u)$, which implies that u solves the Dirichlet boundary-value problem for the Euler-Lagrange equation

$$\mathrm{div}\,\big([F^{**}]'_s(x,\nabla u)\big) = G'_u(x,u), \qquad u|_{\partial\Omega} = u_{\rm D}. \tag{3.10}$$

The nonlinear operator corresponding to (3.10) is monotone, which can be seen from the estimate

$$\begin{aligned} &\int_\Omega \big([F^{**}]'_s(x,\nabla u_1) - [F^{**}]'_s(x,\nabla u_2)\big)\cdot\nabla(u_1-u_2) \\ &\quad + \big(G'_u(x,u_1) - G'_u(x,u_2)\big)(u_1-u_2)\,\mathrm{d}x \geq \left(\frac{1}{\ell_1} + \gamma\right) ||u_1-u_2||^2_{L^2(\Omega)} \geq 0, \end{aligned} \tag{3.11}$$

where (3.6) and (3.8) have been used. Therefore, the potential of (3.10), i.e. the functional $u \mapsto \int_\Omega F^{**}(x,\nabla u) + G(x,u)\,\mathrm{d}x$, is convex on $\{u \in W^{1,p}(\Omega);\ u|_{\partial\Omega} = u_{\rm D}\}$.

This implies that u minimizes this potential on $W^{1,p}(\Omega)$ under the condition $u|_{\partial\Omega} = u_{\rm D}$. Then it suffices to take $\nu \in \mathcal{Y}^p(\Omega;\mathbb{R}^n)$ such that

$$F^{**}(x,\nabla u) = \int_{\mathbb{R}^n} F(x,s)\nu_x(\mathrm{d}s) \qquad \text{and} \qquad \int_{\mathbb{R}^n} s\nu_x(\mathrm{d}s) = \nabla u(x) \tag{3.12}$$

for a.a. $x \in \Omega$. Such ν does exist due to the definition of the convex envelope $F^{**}(x,\cdot)$ and due to the Carathéodory property of F (hence F^{**} is a Carathéodory integrand), the set-valued mapping $x \mapsto \{\nu_x \in M_1^+(\mathbb{R}^n);\ (3.12)\text{ holds}\}$ is measurable and admits therefore a weak* measurable selection $x \mapsto \nu_x$; see [42, Proof of Proposition 3.1.9] for similar arguments. Moreover, the integrability of $\int_{\mathbb{R}^n} |s|^p \nu_x(\mathrm{d}s)$ required in (2.1) follows from coercivity (2.2) of F and the fact that $\int_\Omega \int_{\mathbb{R}^n} F(x,s)\nu_x(\mathrm{d}s)\,\mathrm{d}x$ is finite. $\square$

The constants c_4 in (3.1), ℓ_G in (3.2), as well as D_{Ω,s^*} in (3.5) can be assumed to be explicitly at our disposal (see Section 6). Then, by standards arguments, we can state an a-priori estimate in terms of $\|u^{(0)} - u\|_{L^2(\Omega)}$ (the adjective "a-priori" refers here to that both the solution u can be estimated a-priori by $||u_{\rm D}||_{W^{1-1/p,p}(\partial\Omega)}$ and the initial iteration $u^{(0)}$ is chosen a-priori) and an a-posteriori estimate in terms of $\|u^{(k+1)} - u^{(k)}\|_{L^2(\Omega)}$:

Proposition 3.4. *Let* (2.2), (2.3), *and* (3.1)–(3.3), (3.8) *and* (3.9) *be valid, and let* (u,ν) *be a solution to* $(\mathfrak{RP})$. *Then, for each* $j \geq 0$ *there holds*

$$||u^{(j)} - u||_{L^2(\Omega)} \leq \ell_2^j\, ||u^{(0)} - u||_{L^2(\Omega)}. \tag{3.13}$$

Let $(u^{(k+1)},\nu^{(k+1)})$ *be the output of Algorithm* $(\mathcal{A}_{\rm FP})$. *There holds*

$$||u^{(k+1)} - u||_{L^2(\Omega)} \leq \varepsilon_{\rm FP} \frac{\ell_2}{1-\ell_2}. \tag{3.14}$$

Remark 3.5. One cannot expect any convergence of $\{\nu^{(k)}\}_{k\in\mathbb{N}}$ because ν constructed in (3.12) need not be determined uniquely. In some particular situations, however, one can prove convergence of the Young measure support and weak convergence of volume fractions [4, 11]. Also, incorporating an estimate (4.7) below, we deduce convergence of "stresses" in the sense

$$\|[F^{**}]'_s(\cdot,\nabla u^{(k+1)}) - [F^{**}]'_s(\cdot,\nabla u^{(k)})\|^{\varrho}_{L^{p'}(\Omega;\mathbb{R}^n)} \leq C\|u^{(k)} - u^{(k-1)}\|^2_{L^2(\Omega)}. \tag{3.15}$$

Remark 3.6. If ν-component is forgotten, the iteration of Algorithm $(\mathcal{A}_{\rm FP})$ can be written as: Find $u^{(k+1)} \in W^{1,p}(\Omega)$, $u|_{\partial\Omega} = u_{\rm D}$, such that, for all $v \in W^{1,p}(\Omega)$, $v|_{\partial\Omega} = 0$, there holds

$$\int_\Omega [F^{**}]'_s(x,\nabla u^{(k+1)}) \cdot \nabla v\,\mathrm{d}x = -\int_\Omega G'_u(x,u^{(k)})v\,\mathrm{d}x \tag{3.16}$$

(see also Lemma 4.1 below). Since we did not want to include F^{**} in the computations, we defined the iteration by a minimization problem involving also ν.

Remark 3.7. The assumptions (3.1) and (3.3) involve F^{**} whose explicit knowledge is, however, rather exceptional; the examples in Sections 6 or 7 are such an exception. Extreme difficulties in explicit evaluation of F^{**} even in very special case can be seen in [7, 11, 18]. It should be emphasized that (3.3) can be deduced from (2.2). Unfortunately, it is not obvious whether (3.1) can be verified without explicit knowledge of F^{**}. However, it should be amphasized that (3.1) is not needed for the implementation of Algorithm $(\mathcal{A}_{\rm FP})$ and whenever the Algorithm converges, it converges ultimately to a solution of $(\mathfrak{RP})$; hence, it is worth trying numerical usage of the Algorithm even if (3.1) is not verified in a particular case in question.

Besides, even if F^{**} is explicitly known so that one can think about minimizing $u \mapsto \int_\Omega F^{**}(x,\nabla u) + G(x,u)\,\mathrm{d}x$ which is algorithmically "cheaper" than solving $(\mathfrak{RP})$, the Young-measure solution contains more information than pure knowledge of the underlying "deformation" u so the effort made by implementing a "more expensive" algorithm is not completely lost; cf. e.g. [15, 18, 39] for usage of Young measures to construct minimizing sequences in this or similar circumstances. Moreover, Algorithm $(\mathcal{A}_{\rm FP})$ circumvents difficulties arising from degenerate convexity (i.e., lacking uniform strict convexity) of F^{**}.

4. Discretization of $(\mathfrak{RP}^{(k)})$

The fairly general construction of finite-dimensional convex subsets of $\mathcal{Y}^p(\Omega;\mathbb{R}^n)$ has been performed rigourously in [13, 32, 40, 41, 42] by using systematically duality arguments. Referring to these works, we present briefly the resulting discretization of $(\mathfrak{RP}^{(k)})$.

4.1. **The basic construction and discrete optimality conditions.** For a discretization of the polyhedral (polygonal if $n=2$) bounded Lipschitz domain $\Omega\subset\mathbb{R}^n$, let us consider a regular triangulation $\mathcal{T}$ of Ω. We will refer to $\mathcal{T}$ rather through its mesh parameter $h:=\max_{T\in\mathcal{T}}\mathrm{diam}(T)$. We set

$$V_h(\Omega) := \{v_h\in W^{1,\infty}(\Omega);\ \forall T\in\mathcal{T}:\ v_h|_T \text{ affine}\}, \tag{4.1}$$

$$L_h(\Omega) := \{p_h\in L^{\infty}(\Omega);\ \forall T\in\mathcal{T}:\ p_h|_T \text{ constant}\}. \tag{4.2}$$

The notations $V_h(\Omega;\mathbb{R}^n)$ and $L_h(\Omega;\mathbb{R}^n)$ for $\mathbb{R}^n$-valued functions will be used, too. By $\mathcal{I}_\mathcal{T}: C(\overline{\Omega})\to V_h(\Omega)$ we denote the nodal interpolation operator associated to $\mathcal{T}$ and we define a function $h_\mathcal{T}\in L_h(\Omega)$ by $h_\mathcal{T}|_T:=\mathrm{diam}(T)$ for all $T\in\mathcal{T}$.

Let us assume, for simplicity, uniform $W^{1,\infty}$-estimates for all discrete solutions and let us consider a sufficiently large but bounded, polyhedral, convex set $\omega\subset\mathbb{R}^n$ where all gradients of discrete solutions will live. This seems in accord with our example in Sect. 6, otherwise we would have additionally to make a limit passage with ω to $\mathbb{R}^n$ as in [13, Proposition 2]. Furthermore, we consider a regular triangulation τ of ω with nodes $\mathcal{N}_\tau$ and will refer to τ rather through its mesh parameter $d:=\max_{T\in\tau}\mathrm{diam}(T)$.

We define

$$\mathcal{Y}_{d,h}(\Omega;\mathbb{R}^n) := \Big\{\nu\in\mathcal{Y}^p(\Omega;\mathbb{R}^n);\ \forall T\in\mathcal{T}\ \ \forall s\in\mathcal{N}_\tau\ \ \exists\theta_s^T\in[0,1]: \\ \sum_{s\in\mathcal{N}_\tau}\theta_s^T=1,\ \ \nu|_T=\sum_{s\in\mathcal{N}_\tau}\theta_s^T\delta_s\Big\}.$$

The closed convex set $\mathcal{Y}_{d,h}(\Omega;\mathbb{R}^n)$ consists of all $\mathcal{T}$-elementwise homogeneous L^p-Young measures which are supported in the nodes of τ.

Given an approximation $u_{d,h}^{(k-1)}$ of $u^{(k-1)}$, the set $\mathcal{Y}_{d,h}(\Omega;\mathbb{R}^n)$ allows for an immediate discretization of $(\mathfrak{RP}^{(k)})$:

$$(\mathfrak{RP}_{d,h}^{(k)})\quad\left\{\begin{array}{ll}\text{Minimize} & \bar\Phi_{d,h}^{(k)}(u_{d,h},\nu_{d,h}) := \displaystyle\int_\Omega\bigg(\int_{\mathbb{R}^n}F(x,s)\,[\nu_{d,h}]_x(\mathrm{d}s) \\ & \qquad\qquad + G_u'(x,u_{d,h}^{(k-1)})(u_{d,h}-u_{d,h}^{(k-1)})\bigg)\mathrm{d}x, \\ \text{subject to} & \displaystyle\int_{\mathbb{R}^n}s[\nu_{d,h}]_x(\mathrm{d}s)=\nabla u_{d,h}(x)\quad\text{for a.a. } x\in\Omega, \\ & u_{d,h}\in V_h(\Omega),\quad \nu_{d,h}\in\mathcal{Y}_{d,h}(\Omega;\mathbb{R}^n),\quad u_{d,h}|_{\partial\Omega}=\mathcal{I}_\mathcal{T}u_{\rm D}|_{\partial\Omega}.\end{array}\right.$$

Existence of a solution $(u_{d,h}^{(k)}, \nu_{d,h}^{(k)})$ to $(\mathfrak{RP}_{d,h}^{(k)})$ is guaranteed if $(\mathfrak{RP}_{d,h}^{(k)})$ is feasible. Optimality conditions, invented in [42], are the key towards an error analysis and an efficient implementation of $(\mathfrak{RP}_{d,h}^{(k)})$.

Lemma 4.1. (See [42, Proposition 5.5.3].) *Let $(u_{d,h}^{(k)}, \nu_{d,h}^{(k)}) \in V_h(\Omega) \times \mathcal{Y}_{d,h}(\Omega;\mathbb{R}^n)$ be such that, for almost all $x \in \Omega$, there holds $\nabla u_{d,h}^{(k)}(x) \in \operatorname{int}(\omega)$. Then the pair $(u_{d,h}^{(k)}, \nu_{d,h}^{(k)})$ is a solution to $(\mathfrak{RP}_{d,h}^{(k)})$ if and only if it is feasible for $(\mathfrak{RP}_{d,h}^{(k)})$ and there exists $\lambda_{d,h}^{(k)} \in L_h(\Omega;\mathbb{R}^n)$ such that, for almost all $x \in \Omega$, we have*

$$\max_{s' \in \mathcal{N}_\tau} \big(\lambda_{d,h}^{(k)}(x) \cdot s' - F(x,s')\big) = \int_{\mathbb{R}^n} \lambda_{d,h}^{(k)}(x) \cdot s - F(x,s)[\nu_{d,h}^{(k)}]_x(\mathrm{d}s), \tag{4.3}$$

and, for all $v_h \in V_h(\Omega)$ with $v_h|_{\partial\Omega} = 0$, there holds

$$\int_\Omega \lambda_{d,h}^{(k)} \cdot \nabla v_h \,\mathrm{d}x + \int_\Omega G_u'(x, u_{d,h}^{(k-1)})\, v_h \,\mathrm{d}x = 0. \tag{4.4}$$

Remark 4.2. The problem $(\mathfrak{RP}_{d,h}^{(k)})$ has a structure of a minimization problem with a linear cost functional, linear constraints, and a convex set of admissible pairs $(u_{d,h}, \nu_{d,h})$, and (4.3)–(4.4) are just conventional *Karush-Kuhn-Tucker optimality conditions* modified to this concrete case. The function $\lambda_{d,h}^{(k)}$ is the *Lagrange multiplier* for the constraint $\nabla u_{d,h}|_T = \int_{\mathbb{R}^n} s\nu_{d,h}|_T(\mathrm{d}s)$, $T \in \mathcal{T}$, involved in $(\mathfrak{RP}_{d,h}^{(k)})$.

Any solution $(u_{d,h}^{(k)}, \nu_{d,h}^{(k)})$ to $(\mathfrak{RP}_{d,h}^{(k)})$ is still a solution to $(\mathfrak{RP}_{d,h}^{(k)})$ modified by replacing $F(x,\cdot)$ by the convex hull of its nodal interpolant F_d on τ, $F_d(x,\cdot) := \mathcal{I}_\tau F(x,\cdot)$; we put $F_d(x,\cdot) = +\infty$ in $\mathbb{R}^n \setminus \overline{\omega}$. Thus we can state the following lemma in which $\partial_s[F_d^{**}]$ denotes the subgradient of the convex, continuous, τ-piecewise affine function $F_d^{**}(x,s)$ with respect to s.

Lemma 4.3. (See [4, 13].) *Assume that $(u_{d,h}^{(k)}, \nu_{d,h}^{(k)})$ is a solution to $(\mathfrak{RP}_{d,h}^{(k)})$ and $\lambda_{d,h}^{(k)} \in L_h(\Omega;\mathbb{R}^n)$ satisfies the conditions of Lemma 4.1. Then, for almost all $x \in \Omega$, it holds*

$$\lambda_{d,h}^{(k)}(x) \in \partial_s[F_d^{**}](x, \nabla u_{d,h}^{(k)}(x)).$$

If for almost all $x \in \Omega$ the mappings $F(x,\cdot)$ and $F^{**}(x,\cdot)$ are of class $C_{loc}^{1,1}$ and if $\big(F(x,\cdot)|_\omega\big)^{**} = \big(F^{**}(x,\cdot)\big)|_\omega$ then there holds

$$\big\|\lambda_{d,h}^{(k)} - [F^{**}]_s'(\cdot, \nabla u_{d,h}^{(k)})\big\|_{L^{p'}(\Omega;\mathbb{R}^n)} \le c_6 d \,\big\|[F^{**}]_s''\big\|_{L^\infty(\Omega\times\omega;\mathbb{R}^{n\times n})}. \tag{4.5}$$

Remark 4.4.

(i) The condition $F(x,\cdot), F^{**}(x,\cdot) \in C_{loc}^{1,1}$ can be weakened to $F(x,\cdot), F^{**}(x,\cdot) \in C_{loc}^{1,\alpha}$ for some $\alpha \in (0,1]$. We then have to replace d in (4.5) by d^α.

(ii) Sufficient conditions for $F^{**}(x,\cdot) \in C_{loc}^{1,\alpha}$ and explicit estimates for $||[F^{**}]_s''(x,\cdot)||_{C^{1,\alpha}(B_r(0))}$ are given in [23, 3].

(iii) The proof of Lemma 4.3 uses the fact that ω is discretized into triangles or tetrahedra so that nodal values are extremal values.

4.2. **An a-priori error estimate.** To estimate the error $u_{d,h}^{(k)} - u^{(k)}$ for solutions $u_{d,h}^{(k)}$ and $u^{(k)}$ to $(\mathfrak{RP}_{d,h}^{(k)})$ and $(\mathfrak{RP}^{(k)})$, respectively, we employ the auxiliary problem $(\mathfrak{AP}_{\bar u})$ introduced in Section 3 but with $u_{d,h}^{(k-1)}$ in place of $\bar u$. According to Lemma 3.1 there holds for solutions $(\tilde u^{(k)}, \tilde\nu^{(k)})$ to $(\mathfrak{AP}_{u_{d,h}^{(k-1)}})$ and $(u^{(k)}, \nu^{(k)})$ to $(\mathfrak{RP}^{(k)})$,

$$\|\tilde u^{(k)} - u^{(k)}\|_{L^2(\Omega)} \le \ell_G \|u_{d,h}^{(k-1)} - u^{(k-1)}\|_{L^2(\Omega)}. \tag{4.6}$$

Combining the optimality conditions of Lemma 4.1 with the estimates of Lemma 4.3, (4.6), and the Euler-Lagrange equations for the solution $u^{(k)}$ to $(\mathfrak{RP}^{(k)})$, one can prove the error estimate of Proposition 4.5 below. Some arguments in the proof are similar to those in [4, 11]. The focus of the result presented here is the right scaling of d, h, and k. Some notation is necessary to estimate the error caused by the approximation of non-homogeneous boundary data.

Let $\mathcal{E}(\mathcal{T})$ denote the set of sides (=edges if $n=2$ or faces if $n=3$) in $\mathcal{T}$, and let $h_{\mathcal{E}} \in L^\infty(\cup\mathcal{E}(\mathcal{T}))$ be defined by $h_{\mathcal{E}}|_E := h_E := \operatorname{diam}(E)$ for $E \in \mathcal{E}(\mathcal{T})$. For $\phi \in C(\partial\Omega)$ satisfying $\phi|_E \in W^{2,2}(E)$ for all $E \in \mathcal{E}(\mathcal{T})$ with $E \subset \partial\Omega$, let $\partial^2_{\mathcal{E}}\phi/\partial s^2$ denote the sidewise second derivative of ϕ on $\partial\Omega$.

Proposition 4.5. *Assume that there exist* $1 < \varrho \le 2$, $0 \le \sigma < \infty$, *and* $c_7 > 0$ *such that, for almost all* $x \in \Omega$ *and all* $s_1, s_2 \in \mathbb{R}^n$, *there holds*

$$
\tag{4.7}
\begin{aligned}
|[F^{**}]'_s(x,s_1) - [F^{**}]'_s(x,s_2)|^\varrho \le\ & c_7\left(1 + |s_1|^\sigma + |s_2|^\sigma\right)\\
&\times\left([F^{**}]'_s(x,s_1) - [F^{**}]'_s(x,s_2)\right)\cdot(s_1 - s_2).
\end{aligned}
$$

Suppose that the conditions of Lemma 4.1 and Lemma 4.3 are satisfied and $u_{\mathrm{D}} \in C(\overline{\Omega})$ *is such that* $u_{\mathrm{D}}|_E \in W^{2,2}(E)$ *for all* $E \in \mathcal{E}(\mathcal{T})$ *with* $E \subset \partial\Omega$. *Moreover, let* $(\tilde{u}^{(k)}, \tilde{\nu}^{(k)})$ *be a solution to* $(\mathfrak{AP}_{u_{d,h}^{(k-1)}})$. *Then, there holds*

$$
\begin{aligned}
\|u^{(k)} - u^{(k)}_{d,h}\|^2_{L^2(\Omega)} \le C_1 \Big(& \inf_{\substack{w_h \in V_h(\Omega),\\ w_h|_{\partial\Omega} = \mathcal{I}_{\mathcal{T}} u_{\mathrm{D}}|_{\partial\Omega}}} \|\nabla(\tilde{u}^{(k)} - w_h)\|^{\varrho'}_{L^p(\Omega;\mathbb{R}^n)} + \|u^{(k-1)} - u^{(k-1)}_{d,h}\|^2_{L^2(\Omega)}\\
&+ \Big\| h_{\mathcal{E}}^{3/2} \frac{\partial^2_{\mathcal{E}} u_{\mathrm{D}}}{\partial s^2}\Big\|^2_{L^2(\partial\Omega;\mathbb{R}^{(n-1)\times(n-1)})} + d\,\big\|[F^{**}]''_s\big\|_{L^\infty(\Omega\times\omega;\mathbb{R}^{n\times n})}\Big).
\end{aligned}
$$

The constant $C_1 > 0$ *is independent of* k *and the triangulations* $\mathcal{T}$ *and* τ *but depends on an a-priori bound for* $\|\nabla\tilde{u}^{(k)}\|_{L^p(\Omega)} + \|\nabla u^{(k)}_{d,h}\|_{L^p(\Omega)}$.

Proof. Let $v \in W^{1,p}(\Omega)$ satisfy $v|_{\partial\Omega} = (\mathcal{I}_{\mathcal{T}} u_{\mathrm{D}} - u_{\mathrm{D}})|_{\partial\Omega}$. The triangle inequality and the fine version of Poincaré's inequality, cf. (3.6), yield

$$
\begin{aligned}
\|u^{(k)}_{d,h} - u^{(k)}\|_{L^2(\Omega)} &\le \|u^{(k)}_{d,h} - \tilde{u}^{(k)} - v\|_{L^2(\Omega)} + \|v\|_{L^2(\Omega)} + \|\tilde{u}^{(k)} - u^{(k)}\|_{L^2(\Omega)}\\
&\le D^{1/2}_{\Omega,s^*}\, \|s^*\cdot\nabla(u^{(k)}_{d,h} - \tilde{u}^{(k)} - v)\|_{L^2(\Omega)} + \|v\|_{L^2(\Omega)} + \|\tilde{u}^{(k)} - u^{(k)}\|_{L^2(\Omega)}\\
&\le D^{1/2}_{\Omega,s^*}\, \|s^*\cdot\nabla(u^{(k)}_{d,h} - \tilde{u}^{(k)})\|_{L^2(\Omega)} + c_8\|v\|_{W^{1,2}(\Omega)} + \|\tilde{u}^{(k)} - u^{(k)}\|_{L^2(\Omega)};
\end{aligned}
$$

we used that $u^{(k)}_{d,h} - \tilde{u}^{(k)} - v$ vanishes on $\partial\Omega$. A result in [6] shows that we can choose v such that

$$
\|v\|_{W^{1,2}(\Omega)} \le c_9 \Big\| h_{\mathcal{E}}^{3/2} \frac{\partial^2_{\mathcal{E}} u_{\mathrm{D}}}{\partial s^2}\Big\|_{L^2(\partial\Omega;\mathbb{R}^{(n-1)\times(n-1)})}.
$$

Employing (4.6) we thus have

$$
\tag{4.8}
\begin{aligned}
\|u^{(k)}_{d,h} - u^{(k)}\|_{L^2(\Omega)} &\le D^{1/2}_{\Omega,s^*}\, \|s^*\cdot\nabla(u^{(k)}_{d,h} - \tilde{u}^{(k)})\|_{L^2(\Omega)}\\
&+ c_8 c_9 \Big\| h_{\mathcal{E}}^{3/2} \frac{\partial^2_{\mathcal{E}} u_{\mathrm{D}}}{\partial s^2}\Big\|_{L^2(\partial\Omega;\mathbb{R}^{(n-1)\times(n-1)})} + \ell_2\|u^{(k-1)}_{d,h} - u^{(k-1)}\|_{L^2(\Omega)}.
\end{aligned}
$$

Assumption (3.1) implies

$$
\tag{4.9}
\begin{aligned}
&\frac{c_4}{2}\|s^*\cdot\nabla(u^{(k)}_{d,h} - \tilde{u}^{(k)})\|^2_{L^2(\Omega)}\\
&\le \frac{1}{2}\int_\Omega \left([F^{**}]'_s(x,\nabla u^{(k)}_{d,h}) - [F^{**}]'_s(x,\nabla\tilde{u}^{(k)})\right)\cdot\nabla(u^{(k)}_{d,h} - \tilde{u}^{(k)})\,\mathrm{d}x.
\end{aligned}
$$

Following the argumentation in [11, Proof of Theorem 2] we deduce from (4.7) that

$$\begin{aligned}(4.10)\qquad &\frac{1}{2c_{10}}\|[F^{**}]'_s(\cdot,\nabla u_{d,h}^{(k)}) - [F^{**}]'_s(\cdot,\nabla\tilde{u}^{(k)})\|^{\varrho}_{L^{p'}(\Omega;\mathbb{R}^n)}\\ &\quad\le \frac{1}{2}\int_\Omega \big([F^{**}]'_s(x,\nabla u_{d,h}^{(k)}) - [F^{**}]'_s(x,\nabla\tilde{u}^{(k)})\big)\cdot\nabla(u_{d,h}^{(k)}-\tilde{u}^{(k)})\,\mathrm{d}x\end{aligned}$$

where $c_{10} > 0$ is independent of $\mathcal{T}$ and τ but involves the a-priori bound

$$\|\nabla\tilde{u}^{(k)}\|_{L^p(\Omega;\mathbb{R}^n)} + \|\nabla u_{d,h}^{(k)}\|_{L^p(\Omega;\mathbb{R}^n)} \le c_{11}$$

which follows from (2.2). Inserting $\lambda_{d,h}^{(k)}$ and employing Hölder's inequality, Lemma 4.3, and the a-priori bound c_{11}, we infer

$$\begin{aligned}(4.11)\;&\int_\Omega ([F^{**}]'_s(x,\nabla u_{d,h}^{(k)}) - [F^{**}]'_s(x,\nabla\tilde{u}^{(k)}))\cdot\nabla(u_{d,h}^{(k)}-\tilde{u}^{(k)})\,\mathrm{d}x\\ &\le \int_\Omega \big(\lambda_{d,h}^{(k)} - [F^{**}]'_s(x,\nabla\tilde{u}^{(k)})\big)\cdot\nabla(u_{d,h}^{(k)}-\tilde{u}^{(k)})\,\mathrm{d}x\\ &\quad+\|[F^{**}]'_s(\cdot,\nabla u_{d,h}^{(k)}) - \lambda_{d,h}^{(k)}\|_{L^{p'}(\Omega;\mathbb{R}^n)}\|\nabla(u_{d,h}^{(k)}-\tilde{u}^{(k)})\|_{L^p(\Omega;\mathbb{R}^n)}\\ &\le \int_\Omega \Big(\lambda_{d,h}^{(k)} - [F^{**}]'_s(x,\nabla\tilde{u}^{(k)})\Big)\cdot\nabla(u_{d,h}^{(k)}-\tilde{u}^{(k)})\,\mathrm{d}x + c_6c_{11}d\,\|[F^{**}]''_s\|_{L^\infty(\Omega\times\omega;\mathbb{R}^{n\times n})}.\end{aligned}$$

The Euler-Lagrange equations for $\tilde{u}^{(k)}$, Lemma 4.1, and Hölder's inequality prove, for arbitrary $v_h \in V_h(\Omega) \subset W^{1,p}(\Omega)$ with $v_h|_{\partial\Omega} = 0$,

$$\begin{aligned}(4.12)\qquad &\int_\Omega \big(\lambda_{d,h}^{(k)} - [F^{**}]'_s(x,\nabla\tilde{u}^{(k)})\big)\cdot\nabla(u_{d,h}^{(k)}-\tilde{u}^{(k)})\,\mathrm{d}x\\ &\quad= \int_\Omega \big(\lambda_{d,h}^{(k)} - [F^{**}]'_s(x,\nabla\tilde{u}^{(k)})\big)\cdot\nabla(u_{d,h}^{(k)}-\tilde{u}^{(k)}-v_h)\,\mathrm{d}x\\ &\quad\le \|\lambda_{d,h}^{(k)} - [F^{**}]'_s(\cdot,\nabla\tilde{u}^{(k)})\|_{L^{p'}(\Omega;\mathbb{R}^n)}\,\|\nabla(u_{d,h}^{(k)}-\tilde{u}^{(k)}-v_h)\|_{L^p(\Omega;\mathbb{R}^n)}.\end{aligned}$$

The triangle inequality and Lemma 4.3 yield

$$\begin{aligned}(4.13)\quad &\|\lambda_{d,h}^{(k)} - [F^{**}]'_s(\cdot,\nabla\tilde{u}^{(k)})\|_{L^{p'}(\Omega;\mathbb{R}^n)}\\ &\le \|[F^{**}]'_s(\cdot,\nabla u_{d,h}^{(k)}) - [F^{**}]'_s(\cdot,\nabla\tilde{u}^{(k)})\|_{L^{p'}(\Omega;\mathbb{R}^n)} + c_6d\|[F^{**}]''_s\|_{L^\infty(\Omega\times\omega;\mathbb{R}^{n\times n})}.\end{aligned}$$

Employing (4.13) in (4.12) and Young's inequality $ab \le a^\varrho/\varrho + b^{\varrho'}/\varrho'$ for certain $a, b \ge 0$ shows

$$\begin{aligned}(4.14)\;&\int_\Omega \big(\lambda_{d,h}^{(k)} - [F^{**}]'_s(x,\nabla\tilde{u}^{(k)})\big)\cdot\nabla(u_{d,h}^{(k)}-\tilde{u}^{(k)})\,\mathrm{d}x\\ &\le \frac{1}{2c_{10}\varrho}\,\|[F^{**}]'_s(\cdot,\nabla u_{d,h}^{(k)}) - [F^{**}]'_s(\cdot,\nabla\tilde{u}^{(k)})\|^{\varrho}_{L^{p'}(\Omega;\mathbb{R}^n)}\\ &\quad+\Big(1+\frac{(2c_{10})^{\varrho'/\varrho}}{\varrho}\Big)\|\nabla(u_{d,h}^{(k)}-\tilde{u}^{(k)}-v_h)\|^{\varrho'}_{L^p(\Omega;\mathbb{R}^n)} + c_6^\varrho d^\varrho\|[F^{**}]''_s\|^\varrho_{L^\infty(\Omega\times\omega;\mathbb{R}^{n\times n})}.\end{aligned}$$

The combination of (4.9)–(4.11) with (4.14) yields, after absorbing $1/(2c_{10}\varrho)\,\|[F^{**}]'_s(\cdot,\nabla u_{d,h}^{(k)}) - [F^{**}]'_s(\cdot,\nabla\tilde{u}^{(k)})\|^{\varrho}_{L^{p'}(\Omega;\mathbb{R}^n)}$ on the right-hand side,

$$\begin{aligned}&\frac{\varrho-1}{2c_{10}\varrho}\|[F^{**}]'_s(\cdot,\nabla u_{d,h}^{(k)}) - [F^{**}]'_s(\cdot,\nabla\tilde{u}^{(k)})\|^{\varrho}_{L^{p'}(\Omega;\mathbb{R}^n)} + \frac{c_4}{2}\|s^*\cdot\nabla(u_{d,h}^{(k)}-\tilde{u}^{(k)})\|^2_{L^2(\Omega)}\\ &\quad\le \Big(1+\frac{(2c_{10})^{\varrho'/\varrho}}{\varrho}\Big)\inf_{v_h\in V_h(\Omega), v_h|_{\partial\Omega}=0}\|\nabla(u_{d,h}^{(k)}-\tilde{u}^{(k)}-v_h)\|^{\varrho'}_{L^p(\Omega;\mathbb{R}^n)}\\ &\qquad+c_6c_{11}d\|[F^{**}]''_s\|_{L^\infty(\Omega\times\omega;\mathbb{R}^{n\times n})} + c_6^\varrho d^\varrho\|[F^{**}]''_s\|^\varrho_{L^\infty(\Omega\times\omega;\mathbb{R}^{n\times n})}.\end{aligned}$$

Using this estimate in (4.8), choosing $v_h = w_h - u_{d,h}^{(k)}$ for arbitrary $w_h \in V_h(\Omega)$ with $w_h|_{\partial\Omega} = \mathcal{I}_{\mathcal{T}}u_{\mathrm{D}}|_{\partial\Omega}$, and estimating $d^\varrho\|[F^{**}]''_s\|^\varrho_{L^\infty(\Omega\times\omega;\mathbb{R}^{n\times n})} \le c_{12}d\|[F^{**}]''_s\|_{L^\infty(\Omega\times\omega;\mathbb{R}^{n\times n})}$ since $\varrho > 1$ and $d \le c_{13}$, proves the proposition. $\square$

A simple induction argument proves an estimate for the error $\|u_{d,h}^{(k)}-u\|_{L^2(\Omega)}$.

Theorem 4.6. *Under the same conditions of Proposition 4.5 there holds*

$$\|u-u_{d,h}^{(k)}\|_{L^2(\Omega)}^2 \le C_2\Bigg(\ell_2^{2k}\,\|u-u^{(0)}\|_{L^2(\Omega)}^2+\sum_{j=1}^{k}\inf_{\substack{w_h\in V_h(\Omega),\\ w_h|_{\partial\Omega}=\mathcal{I}_{\mathcal{T}}u_{\mathrm{D}}|_{\partial\Omega}}}\|\nabla(\tilde u^{(j)}-w_h)\|_{L^p(\Omega;\mathbb{R}^n)}^{\varrho'}$$
$$+\|u^{(0)}-u_{d,h}^{(0)}\|_{L^2(\Omega)}^2+k\left(d\|[F^{**}]_s''\|_{L^\infty(\Omega\times\omega;\mathbb{R}^{n\times n})}+\left\|h_{\mathcal{E}}^{3/2}\frac{\partial_{\mathcal{E}}^2u_{\mathrm{D}}}{\partial s^2}\right\|_{L^2(\partial\Omega;\mathbb{R}^{(n-1)\times(n-1)})}^2\right)\Bigg).$$

Proof. The triangle inequality and Proposition 3.4 show

$$\|u-u_{d,h}^{(k)}\|_{L^2(\Omega)}\ \le\ \ell_2^k\,\|u-u^{(0)}\|_{L^2(\Omega)}+\|u^{(k)}-u_{d,h}^{(k)}\|_{L^2(\Omega)}.$$

Iterated application of Proposition 4.5 proves Theorem 4.6. ☐

A density argument and Theorem 4.6 prove convergence $u_{d,h}^{(k)}\to u$ in $L^2(\Omega)$ for $(d,h)\to 0$ and $k\to\infty$ (for $d,h\ll 1/k$), where d and h are the maximal meshsizes of τ and $\mathcal{T}$, respectively. If $\tilde u^{(j)}$, $j=0,1,2,...,k$, satisfies $\tilde u^{(j)}\in W^{1+\beta,p}(\Omega)$ for some $\beta\in(0,1]$ so that

$$\inf_{\substack{w_h\in V_h(\Omega),\\ w_h|_{\partial\Omega}=\mathcal{I}_{\mathcal{T}}u_{\mathrm{D}}|_{\partial\Omega}}}\|\nabla(\tilde u^{(j)}-w_h)\|_{L^p(\Omega;\mathbb{R}^n)}^{\varrho'/2}\le c_{14}h^\alpha$$

for some $\alpha\in(0,1]$ and $j=0,1,2,...,k$, we may choose $u_{d,h}^{(0)}=\mathcal{I}_{\mathcal{T}}u^{(0)}$, $d=h^{2\alpha}$, and, provided $\ell_2<1$, $\log(h^{\alpha/\log(\ell_2)})\le k\le\log(h^{\alpha/\log(\ell_2)})+1$ to verify

$$\|u-u_{d,h}^{(k)}\|_{L^2(\Omega)}\le C_2'\big(1+\log(h^{\alpha/\log(\ell_2)})\big)\,h^\alpha. \tag{4.15}$$

Remark 4.7. Similarly as in Remark 3.7, explicit knowledge of F^{**} is not needed for (4.5) and the estimate of Theorem 4.6 since explicit bounds for $F^{**}(x,\cdot)''$ are provided in [3] in terms of F only.

4.3. **An a-posteriori error estimate.** Since in general higher regularity is not available or α may be very small in (4.15), a-posteriori error estimates that allow for adaptive mesh refinement could yield improved convergence rates.

Let $\sigma_h\in L_h(\Omega;\mathbb{R}^n)$ and $E\in\mathcal{E}(\mathcal{T})$. For $E\subset\partial\Omega$ set $\big[\sigma_h\big]\cdot n_E:=0$. If $E=T_-\cap T_+$ for $T_-,T_+\in\mathcal{T}$ let $n_E\in\mathbb{R}^n$ be the unit vector perpendicular to E pointing from T_- to T_+ and define

$$\big[\sigma_h\big]\cdot n_E:=\big(\sigma_h|_{T_+}-\sigma_h|_{T_-}\big)\cdot n_E.$$

Theorem 4.8. *Under the same conditions of Proposition 4.5 and if* $G_u'(\cdot,u_{d,h}^{(k-1)})\in W^{1,p'}(\Omega)$ *there holds*

$$\begin{aligned}&\|u^{(k)}-u_{d,h}^{(k)}\|_{L^2(\Omega)}^2+\|\lambda_{d,h}^{(k)}-[F^{**}]_s'(\cdot,\nabla u^{(k)})\|_{L^{p'}(\Omega;\mathbb{R}^n)}^{\varrho}\\ &\le C_3\Big(\sum_{E\in\mathcal{E}(\mathcal{T})}h_E\|\big[\lambda_{d,h}^{(k)}\big]\cdot n_E\|_{L^{p'}(E)}^{p'}\Big)^{1/p'}\\ &+C_4\Bigg(\|u^{(k-1)}-u_{d,h}^{(k-1)}\|_{L^2(\Omega)}^2+\left\|h_{\mathcal{E}}^{3/2}\frac{\partial_{\mathcal{E}}^2u_{\mathrm{D}}}{\partial s^2}\right\|_{L^2(\partial\Omega;\mathbb{R}^{(n-1)\times(n-1)})}^2\\ &+\|h_{\mathcal{T}}^2\nabla G_u'(\cdot,u_{d,h}^{(k-1)})\|_{L^{p'}(\Omega;\mathbb{R}^n)}+d\,\|[F^{**}]_s''\|_{L^\infty(\Omega\times\omega;\mathbb{R}^{n\times n})}\Bigg).\end{aligned} \tag{4.16}$$

The constants $C_3,C_4>0$ are independent of k and the meshsizes of $\mathcal{T}$ and τ but depend on an a-priori bound for $\|\nabla\tilde u^{(k)}\|_{L^p(\Omega;\mathbb{R}^n)}+\|\nabla u_{d,h}^{(k)}\|_{L^p(\Omega;\mathbb{R}^n)}$.

Proof. Arguing as in (4.9)–(4.11) we have, for all $v_h \in V_h(\Omega)$ with $v_h|_{\partial\Omega} = 0$,

$$\frac{c_4}{2}\|\sigma^* \cdot \nabla(u_{d,h}^{(k)} - \tilde{u}^{(k)})\|_{L^2(\Omega)}^2 + \frac{1}{2c_{10}}\,\|[F^{**}]_s'(\cdot,\nabla u_{d,h}^{(k)}) - [F^{**}]_s'(\cdot,\nabla\tilde{u}^{(k)})\|_{L^{p'}(\Omega;\mathbb{R}^n)}^{\varrho}$$
$$\leq \int_\Omega \big(\lambda_{d,h}^{(k)} - [F^{**}]_s'(x,\nabla\tilde{u}^{(k)})\big)\cdot\nabla(u_{d,h}^{(k)} - \tilde{u}^{(k)} - v_h)\,\mathrm{d}x + c_6c_{11}d\,\|[F^{**}]_s''\|_{L^\infty(\Omega\times\omega;\mathbb{R}^{n\times n})}.$$

Inserting $v \in W^{1,p}(\Omega)$ with $v|_{\partial\Omega} = (\mathcal{I}_\mathcal{T} u_\mathrm{D} - u_\mathrm{D})|_{\partial\Omega}$ and employing the Euler-Lagrange equations for $\tilde{u}^{(k)}$ proves

$$\int_\Omega \big(\lambda_{d,h}^{(k)} - [F^{**}]_s'(x,\nabla\tilde{u}^{(k)})\big)\cdot\nabla(u_{d,h}^{(k)} - \tilde{u}^{(k)} - v_h)\,\mathrm{d}x$$
$$= \int_\Omega \lambda_{d,h}^{(k)}\cdot\nabla(u_{d,h}^{(k)} - \tilde{u}^{(k)} - v - v_h)\,\mathrm{d}x + \int_\Omega G_u'(x,u_{d,h}^{(k-1)})(u_{d,h}^{(k)} - \tilde{u}^{(k)} - v - v_h)\,\mathrm{d}x$$
$$+ \int_\Omega \big(\lambda_{d,h}^{(k)} - [F^{**}]_s'(x,\nabla\tilde{u}^{(k)})\big)\cdot\nabla v\,\mathrm{d}x.$$

Arguing as in (4.12)-(4.14) shows

$$\int_\Omega \big(\lambda_{d,h}^{(k)} - [F^{**}]_s'(x,\nabla\tilde{u}^{(k)})\big)\cdot\nabla v\,\mathrm{d}x \leq \Big(1 + \frac{(2c_{10})^{\varrho'/\varrho}}{\varrho'}\Big)\|\nabla v\|_{L^p(\Omega;\mathbb{R}^n)}^{\varrho'}$$
$$+ c_6^\varrho d^\varrho \|[F^{**}]_s''\|_{L^\infty(\Omega\times\omega;\mathbb{R}^{n\times n})}^\varrho + \frac{1}{2c_{10}\varrho}\|[F^{**}]_s'(\cdot,\nabla u_{d,h}^{(k)}) - [F^{**}]_s'(\cdot,\nabla\tilde{u}^{(k)})\|_{L^{p'}(\Omega;\mathbb{R}^n)}^\varrho.$$

A $\mathcal{T}$-elementwise integration by parts, $\operatorname{div}\lambda_{d,h}^{(k)}|_T = 0$, and Hölder and Cauchy inequalities yield

$$\int_\Omega \lambda_{d,h}^{(k)}\cdot\nabla(u_{d,h}^{(k)} - \tilde{u}^{(k)} - v - v_h)\,\mathrm{d}x = \sum_{E\in\mathcal{E}(\mathcal{T})}\int_E \big[\lambda_{d,h}^{(k)}\big]\cdot n_E\,(u_{d,h}^{(k)} - \tilde{u}^{(k)} - v - v_h)\,\mathrm{d}s$$
$$\leq \Big(\sum_{E\in\mathcal{E}(\mathcal{T})} h_E\,\|\big[\lambda_{d,h}^{(k)}\big]\cdot n_E\|_{L^{p'}(E)}^{p'}\Big)^{1/p'}\Big(\sum_{E\in\mathcal{E}(\mathcal{T})} h_E^{1-p}\,\|u_{d,h}^{(k)} - \tilde{u}^{(k)} - v - v_h\|_{L^p(E)}^p\Big)^{1/p}$$

The weak interpolation operator $J : W_0^{1,p}(\Omega) \to V_h(\Omega)\cap W_0^{1,p}(\Omega)$ of [9] satisfies, for $w \in W_0^{1,p}(\Omega)$ and $f \in W^{1,p'}(\Omega)$,

$$\int_\Omega f(w - Jw)\,\mathrm{d}x \leq c_{15}\|h_\mathcal{T}^2\nabla f\|_{L^{p'}(\Omega;\mathbb{R}^n)}\|w\|_{W^{1,p}(\Omega)},$$
$$\sum_{E\in\mathcal{E}(\mathcal{T})} h_E^{1-p}\|(w - Jw)\|_{L^p(E)}^p \leq c_{15}^p\|w\|_{W^{1,p}(\Omega)}^p.$$

Setting $v_h = J(u_{d,h}^{(k)} - \tilde{u}^{(k)} - v)$ and combining the previous estimates shows, after absorbing terms on the right-hand side and using $d \leq c_{13}$,

$$\frac{c_4}{2}\|s^*\cdot\nabla(u_{d,h}^{(k)} - \tilde{u}^{(k)})\|_{L^2(\Omega)}^2 + \frac{\varrho - 1}{2c_{10}\varrho}\,\|[F^{**}]_s'(\cdot,\nabla u_{d,h}^{(k)}) - [F^{**}]_s'(\cdot,\nabla\tilde{u}^{(k)})\|_{L^{p'}(\Omega;\mathbb{R}^n)}^\varrho$$
$$\leq c_{16}\Big(\sum_{E\in\mathcal{E}(\mathcal{T})} h_E\|\big[\lambda_{d,h}^{(k)}\big]\cdot n_E\|_{L^{p'}(E)}^{p'}\Big)^{1/p'}\|u_{d,h}^{(k)} - \tilde{u}^{(k)} - v\|_{W^{1,p}(\Omega)} + c_{17}\Big(\|\nabla v\|_{L^p(\Omega;\mathbb{R}^n)}^{\varrho'}$$
$$+ d\,\|[F^{**}]_s''\|_{L^\infty(\Omega\times\omega;\mathbb{R}^{n\times n})} + \|h_\mathcal{T}^2\nabla G_u'(\cdot,u_{d,h}^{(k-1)})\|_{L^{p'}(\Omega;\mathbb{R}^n)}\|u_{d,h}^{(k)} - \tilde{u}^{(k)} - v\|_{W^{1,p}(\Omega)}\Big).$$

Choosing v as in the proof of Proposition 4.5, employing an a-priori bound for $\|u_{d,h}^{(k)} - \tilde{u}^{(k)} - v\|_{W^{1,p}(\Omega)}$, and using (4.8) proves the asserted estimate for $\|u^{(k)} - u_{d,h}^{(k)}\|_{L^2(\Omega)}$. An application of the estimate

$$\|[F^{**}]_s'(\cdot,\nabla u^{(k)}) - [F^{**}]_s'(\cdot,\nabla\tilde{u}^{(k)})\|_{L^{p'}(\Omega;\mathbb{R}^n)}^\varrho \leq c_{18}\|u^{(k-1)} - u_{d,h}^{(k-1)}\|_{L^2(\Omega)}^2,$$

which follows from (4.7) as (4.6) (cf. (4.10)), concludes the proof. ☐

Remark 4.9. The condition $G_u'(\cdot,\nabla u_{d,h}^{(k-1)}) \in W^{1,p'}(\Omega)$ can be dropped. This results in a computable term which is not necessarily of higher order.

Setting $\eta_E := h_E^{1/p'}\|[\lambda_{d,h}^{(k)}]\cdot n_E\|_{L^{p'}(E)}$ and assuming that $d \ll h$ and for $j = k-1, k$ there holds

$$\|u_{d,h}^{(j)} - u^{(j)}\|^2_{L^2(\Omega)} \ll \|\lambda_{d,h}^{(k)} - [F^{**}]_s'(\cdot, \nabla u^{(k)})\|^{\varrho}_{L^{p'}(\Omega;\mathbb{R}^n)},$$

Theorem 4.8 proves a *reliability*-estimate, with "h.o.t." denoting "higher order terms",

$$\|\lambda_{d,h}^{(k)} - [F^{**}]_s'(\cdot, \nabla u^{(k)})\|_{L^{p'}(\Omega;\mathbb{R}^n)} + \text{h.o.t.} \le C_3 \Big(\sum_{E\in\mathcal{E}(\mathcal{T})} \eta_E^{p'}\Big)^{1/(\varrho p')} =: \eta_{R,R}.$$

The inverse estimation techniques of [47] allow for the converse, *efficiency-*, estimate with a different exponent,

$$\eta_{R,E} := \eta_{R,R}^{\varrho} \le C_3'\|\lambda_{d,h}^{(k)} - [F^{**}]_s'(\cdot, \nabla u^{(k)})\|_{L^{p'}(\Omega;\mathbb{R}^n)} + \text{h.o.t.}$$

The gap between $\eta_{R,E}$ and $\eta_{R,R}$ is known as a *reliability-efficiency-gap* [11]. Under similar assumptions one can show [4]

$$\begin{aligned} C_5 \inf_{\sigma_h\in V_h(\Omega;\mathbb{R}^n)} \|\lambda_{d,h}^{(k)} - \sigma_h\|_{L^{p'}(\Omega;\mathbb{R}^n)} &\le \|\lambda_{d,h}^{(k)} - [F^{**}]_s'(\cdot, \nabla u^{(k)})\|_{L^{p'}(\Omega;\mathbb{R}^n)} + \text{h.o.t.} \\ &\le C_5' \inf_{\sigma_h\in V_h(\Omega;\mathbb{R}^n)} \|\lambda_{d,h}^{(k)} - \sigma_h\|^{1/\varrho}_{L^{p'}(\Omega;\mathbb{R}^n)}. \end{aligned}$$

If $[F^{**}]_s'(\cdot, \nabla u^{(k)})$ is smooth, e.g., in $W^{2,p'}$, we have $C_5 = 1$. Since the computation of the infimum appears too expensive an approximation can be defined through the averaging-operator $\mathcal{A} : L^1(\Omega;\mathbb{R}^n) \to V_h(\Omega;\mathbb{R}^n)$ of [9],

$$\eta_{A,E} = \eta_{A,R}^{\varrho} := \|\lambda_{d,h}^{(k)} - \mathcal{A}\lambda_{d,h}^{(k)}\|_{L^{p'}(\Omega)} \approx \inf_{\sigma_h\in V_h(\Omega;\mathbb{R}^n)} \|\lambda_{d,h}^{(k)} - \sigma_h\|_{L^{p'}(\Omega;\mathbb{R}^n)}.$$

5. Efficient implementation by the active-set strategy

As the dimensionality of $(\mathfrak{RP}_{d,h}^{(k)})$ is usually very high but the optimal Young measure is typically supported only on rather low-dimensional sets, it is certainly desirable to reduce the dimensionality by exploiting a certain a-priori information to put the expectedly "non-active" points out of calculations and also to have a certain reliable a-posteriori information to check whether we did it correctly.

This information comes from the optimality conditions in Lemma 4.1. However, the Hamiltonian $\mathcal{H}(x, s) = \lambda_{d,h}^{(k)}(x)\cdot s - F(x, s)$ appearing in these conditions is usually not known and has to be estimated from previous iterations in an iterative algorithm. Indeed, this adaptivity idea, let us call it *active-set strategy* was proposed and first implemented in [13], and further used in [4, 28, 29, 43]. The iterative algorithm in question is the successive refinement of a triangulation of ω. The active-set strategy was also implemented in [31] where the iterative algorithm arises by the sequential quadratic programming approach.

We briefly recall the central idea for the active-set strategy and refer to [13] and Algorithm $(\mathcal{A}_{\mathcal{T}_0,\Theta,\beta,L,m})$ below for its practical realization to solve $(\mathfrak{RP}_{d,h}^{(k)})$ efficiently.

The support $\operatorname{Supp}\nu$ of $\nu \in \mathcal{Y}^p(\Omega;\mathbb{R}^n)$ is given by

$$\operatorname{Supp}\nu := \big\{(x, s)\in\Omega\times\mathbb{R}^n;\quad s \in \operatorname{supp}\nu_x\big\}$$

where $\operatorname{supp}\nu_x \subset \mathbb{R}^n$ is the support of the probability measure ν_x; $\operatorname{Supp}\nu$ is defined up to a set of zero measure.

Given $A \subset \Omega \times \mathcal{N}_\tau$ we define a subset of $\mathcal{Y}_{d,h}(\Omega;\mathbb{R}^n)$ by

$$\mathcal{Y}_{d,h,A}(\Omega;\mathbb{R}^n) = \big\{\nu \in \mathcal{Y}_{d,h}(\Omega;\mathbb{R}^n); \operatorname{Supp}\nu \subset A\big\}.$$

The lower-dimensional subproblem $(\mathfrak{RP}^{(k)}_{d,h,A})$ is then defined as follows.

$$(\mathfrak{RP}^{(k)}_{d,h,A})\qquad \left\{\begin{array}{ll} \text{Minimize} & \bar\Phi^{(k)}_{d,h}(u_{d,h},\nu_{d,h}) = \displaystyle\int_\Omega \bigg(\int_{\mathbb{R}^n} F(x,s)\,[\nu_{d,h}]_x(\mathrm{d}s) \\ & \qquad\qquad + G'_u(x,u^{(k-1)}_{d,h})(u_{d,h}-u^{(k-1)}_{d,h}) \bigg)\mathrm{d}x, \\ \text{subject to} & \displaystyle\int_{\mathbb{R}^n} s[\nu_{d,h}]_x(\mathrm{d}s) = \nabla u_{d,h}(x) \qquad \text{for a.a. } x\in\Omega, \\ & u_{d,h}|_{\partial\Omega} = \mathcal{I}_{\mathcal{T}} u_{\mathrm{D}}|_{\partial\Omega}, \\ & u_{d,h}\in V_h(\Omega), \quad \nu_{d,h}\in \mathcal{Y}_{d,h,A}(\Omega;\mathbb{R}^n). \end{array}\right.$$

Assume that we are given an approximation $\tilde\lambda_h \in L_h(\Omega;\mathbb{R}^n)$ to the Lagrange multiplier $\lambda^{(k)}_{d,h} \in L_h(\Omega;\mathbb{R}^n)$ occurring in the optimality conditions of Lemma 4.1. If $\tilde\lambda_h$ is close enough to $\lambda^{(k)}_{d,h}$ and if A is defined through $\tilde\lambda_h$ as in the following proposition then any solution to $(\mathfrak{RP}^{(k)}_{d,h,A})$ is a solution to $(\mathfrak{RP}^{(k)}_{d,h})$.

Proposition 5.1. (See [13, Corollary 1].) *Let $(u^{(k)}_{d,h},\nu^{(k)}_{d,h})$ be a solution to $(\mathfrak{RP}^{(k)}_{d,h})$ with corresponding multiplier $\lambda^{(k)}_{d,h}$ and let $\tilde\lambda_h \in L_h(\Omega;\mathbb{R}^n)$. If for $\varepsilon \in L_h(\Omega)$ and all $T\in\mathcal{T}$ there holds*

$$\sup_{s\in\omega} \big|(\lambda^{(k)}_{d,h}-\tilde\lambda_h)|_T\cdot s\,\big| \le \frac12\,\varepsilon|_T$$

and if

$$A = \Big\{(x,s)\in\Omega\times\mathcal{N}_\tau;\ \tilde\lambda_h(x)\cdot s - F(x,s) \ge \max_{s'\in\mathcal{N}_\tau}\big(\tilde\lambda_h(x)\cdot s' - F(x,s')\big) - \varepsilon(x)\Big\},$$

then any solution to $(\mathfrak{RP}^{(k)}_{d,h,A})$ is a solution to $(\mathfrak{RP}^{(k)}_{d,h})$.

Proof. The optimality conditions of Lemma 4.1 guarantee

$$\operatorname{Supp}\nu_{d,h}\subset B := \Big\{(x,s)\in\Omega\times\mathcal{N}_\tau; \lambda^{(k)}_{d,h}\cdot s - F(x,s) = \max_{s'\in\mathcal{N}_\tau}\big(\lambda^{(k)}_{d,h}\cdot s' - F(x,s')\big)\Big\}.$$

Therefore (cf. [13]), it suffices to show $B\subset A$. For almost all $x\in\Omega$ and all $s\in\mathbb{R}^n$ such that $(x,s)\in B$ there holds by assumption on ε and definition of B,

$$\begin{aligned}\tilde\lambda_h(x)\cdot s - F(x,s) &\ge \lambda^{(k)}_{d,h}(x)\cdot s - F(x,s) - \varepsilon(x)/2\\ &= \max_{s'\in\mathcal{N}_\tau}\big(\lambda^{(k)}_{d,h}\cdot s' - F(x,s')\big) - \varepsilon(x)/2\\ &\ge \max_{s'\in\mathcal{N}_\tau}\big(\tilde\lambda_h\cdot s' - F(x,s')\big) - \varepsilon(x).\end{aligned}$$

Hence we have $(x,s)\in A$. □

Given some $\tilde\lambda_h$ we do not know ε in general. We may however choose some positive $\varepsilon\in L_h(\Omega)$, define A as in Proposition 5.1, compute a solution to $(\mathfrak{RP}^{(k)}_{d,h,A})$, verify the optimality conditions of Lemma 4.1, and enlarge ε to repeat this procedure until the optimality conditions are satisfied.

6. Illustrative example: 2D broken extremal

We want to illustrate our algorithm on the so-called Tartar's broken-extremal example [35] which is modified for the multidimensional case like in [11, Sect. 8] or [14, 16]. To be more specific, let us consider $n = 2$, $\Omega := (0,K)^2$ with some $K > 0$

and, for almost all $x \in \Omega$, all $s \in \mathbb{R}^n$, and all $u \in \mathbb{R}$,

$$F(x,s) := |s-a|^2|s+a|^2, \tag{6.1}$$

$$G(x,u) := (u - g(a\cdot x))^2 \quad \text{with} \tag{6.2}$$

$$g(\xi) := -\frac{3}{128}(\xi-\xi_\mathrm{b})^5 - \frac{1}{3}(\xi-\xi_\mathrm{b})^3, \tag{6.3}$$

for $a = (\cos\phi, \sin\phi)$ with $\phi = \pi/6$ and for $\xi_b = 1/2$. Note that (6.1) (when shifted by a constant) fits with (2.2) for $p = 4$.

Then (cf. [35]) the relaxed problem $(\mathfrak{RP})$ has the unique solution

$$u(x) = \begin{cases} g(a\cdot x) & \text{for } a\cdot x \in (0,\xi_\mathrm{b}),\\ \dfrac{(a\cdot x-\xi_\mathrm{b})^3}{24} + (a\cdot x - \xi_\mathrm{b}) & \text{for } a\cdot x \in (\xi_\mathrm{b},\sqrt{2}),\end{cases} \tag{6.4a}$$

$$\nu_x = \begin{cases} \dfrac{1-a\cdot\nabla u(x)}{2}\,\delta_{-a} + \dfrac{1+a\cdot\nabla u(x)}{2}\,\delta_a & \text{for } a\cdot x \in (0,\xi_\mathrm{b}),\\ \delta_{\nabla u(x)} & \text{for } a\cdot x \in (\xi_\mathrm{b},\sqrt{2}),\end{cases} \tag{6.4b}$$

provided we choose the boundary data $u_\mathrm{D} := u|_{\partial\Omega}$ with u just from (6.4a). Here we can take a benefit from an explicit knowledge (6.5) of F^{**} although, as already pointed out in Remarks 3.7 and 4.7, our algorithm itself does not exploit the information (6.5) below.

Lemma 6.1. (See [11, Propositions 1–3].) *Let F be as in* (6.1). *For almost all $x \in \Omega$ and all $s \in \mathbb{R}^n$ there holds*

$$F^{**}(x,s) = \max\{|s|^2-1,0\}^2 + 4\big(|s|^2 - (a\cdot s)^2\big). \tag{6.5}$$

Moreover, for almost all $x \in \Omega$ and all $s_1, s_2 \in \mathbb{R}^n$, we have

$$\begin{aligned} \big|[F^{**}]'_s(x,s_1) - [F^{**}]'_s(x,s_2)\big|^2 \;&\le\; 8\left(1+|s_1|^2+|s_2|^2\right)\\ &\qquad\times\big([F^{**}]'_s(x,s_1) - [F^{**}]'_s(x,s_2)\big)\cdot(s_1-s_2),\\ 8\left(a^\perp\cdot(s_1-s_2)\right)^2 &\le \big([F^{**}]'_s(x,s_1) - [F^{**}]'_s(x,s_2)\big)\cdot(s_1-s_2), \end{aligned}$$

with $a^\perp = (\sin\phi, -\cos\phi)$.

Remark 6.2. For almost all $x \in \Omega$ and all $s \in \mathbb{R}^n$ there holds $F^{**}(x,s) = F(x,s)$ if and only if $|s| \ge 1$. Hence only gradients of modulus ≤ 1 lead to a non-trivial Young measure.

Let us point out that Lemma 6.1 proves $c_4 = 8$ and $s^* = a^\perp$ in (3.1) for F from (6.1) and we have $\ell_G = 2$ in (3.2) for G defined by (6.2), while $D_{\Omega,s^*} \le \sqrt{2}K$ in (3.5). Obviously, (3.8) holds even with $\gamma = 2 > -1/\ell_2$ in as $G(x,\cdot)$ from (6.2) is uniformly convex. Lemma 3.3 therefore ensures convergence of Algorithm $(\mathcal{A}_\mathrm{FP})$ in this case if

$$\ell_2 = \frac{D_{\Omega,s^*}\ell_G}{c_4} \le \frac{K}{2\sqrt{2}} < 1,$$

i.e., if the size K of the square Ω is less than $2\sqrt{2}$. For our numerical experiments we chose $K = 1$.

Furthermore, the convex domain $\omega := (-m,m)^2 \subset \mathbb{R}^2$ is triangulated by uniform triangulations τ with meshsize $d > 0$. More precisely, a uniform triangulation τ of ω with meshsize d can be defined through the nodes

$$\mathcal{N}_\tau := \left\{ s \in \mathbb{R}^2;\ \exists i,j \in \{-M,\dots,M\}:\ s = \left(\frac{im}{M},\frac{jm}{M}\right)\right\}, \tag{6.6}$$

where M is a positive integer satisfying $m/d - 1 \leq M \leq m/d$. The elements in τ are chosen as halved squares with sides of lengths m/M and $\sqrt{2}m/M$.

For parameters $\Theta \in \{0, 1/2\}$, $\beta \in [1, 2]$, a positive number $m \in \mathbb{R}$, a list of positive integers $L = (L(0), L(1), L(2), ...)$, and an initial triangulation $\mathcal{T}_0$ of Ω we used the following algorithm to approximate $(\mathfrak{RP})$ on a sequence of uniformly $(\Theta = 0)$ and adaptively $(\Theta = 1/2)$ refined triangulations $\mathcal{T}_j$, $j = 0, 1, 2, ...$ The algorithm can be employed to any specification of $(\mathfrak{RP})$ (though convergence has to be proved for each situation) and combines adaptive mesh refinement with a nested fixed point iteration and the active set strategy introduced in the preceding sections. The parameter β determines the ratio of the meshsizes of the triangulations of Ω and ω. The sequence of integers L is needed for the realization of the active set strategy. Given $j \geq 0$ and a triangulation $\mathcal{T}_j$ of Ω with N_j nodes the number h_j is defined by $h_j = 1/\sqrt{N_j}$. The algorithm terminates if a suitable stopping criterion is satisfied and then the output is an approximate solution $(u_j, \nu_j) \in V_{h_j}(\Omega) \times \mathcal{Y}_{d_j,h_j}(\Omega; \mathbb{R}^2)$ to $(\mathfrak{RP})$ for some $j \geq 0$ and a triangulation τ_j of $\omega = (-m, m)^2$ with meshsize $d_j = h_j^\beta$.

Algorithm $(\mathcal{A}_{\mathcal{T}_0,\Theta,\beta,L,m})$**.**

(a) Set $j := 0$, $k := 0$, $\ell := 0$, and choose $u_j^{(k)} \in V_{h_j}(\Omega)$ such that $u_j^{(k)}|_{\partial\Omega} = \mathcal{I}_{\mathcal{T}_j} u_D|_{\partial\Omega}$. Choose $\lambda_{j,\ell} \in L_h(\Omega; \mathbb{R}^2)$, set $\varepsilon := \infty$, and $d_{j,\ell} := 2^{L(j)} h_j^\beta$.

(b) Generate a uniform triangulation $\tau_{j,\ell}$ of $\omega = (-m, m)^2$ with meshsize $d_{j,\ell}$ and with nodes $\mathcal{N}_{\tau_{j,\ell}}$ as in (6.6).

(c) Define

$$A := \Big\{(x, s) \in \Omega \times \mathcal{N}_{\tau_{j,\ell}};\ \lambda_{j,\ell}(x) \cdot s - F(x, s) > \max_{s' \in \mathcal{N}_{\tau_{j,\ell}}} \lambda_{j,\ell}(x) \cdot s' - F(x, s') - \varepsilon\Big\}.$$

Enlarge A appropriately to ensure feasibility of $(\mathfrak{RP}_{d_{j,\ell},h_j,A}^{(k+1)})$.

(d) Solve the linear optimization problem $(\mathfrak{RP}_{d_{j,\ell},h_j,A}^{(k+1)})$ to obtain a solution $(\tilde{u}_j, \tilde{\nu}_{j,\ell}) \in V_{h_j}(\Omega) \times \mathcal{Y}_{d_{j,\ell},h_j,A}(\Omega; \mathbb{R}^2)$ and a Lagrange multiplier $\tilde{\lambda}_j \in L_{h_j}(\Omega; \mathbb{R}^2)$.

(e) If, for almost all $x \in \Omega$ and all $s \in \mathcal{N}_{\tau_{j,\ell}}$, it holds

$$\tilde{\lambda}_j(x) \cdot s - F(x, s) \leq \int_{\mathbb{R}^2} \big(\tilde{\lambda}_j(x) \cdot s' - F(x, s')\big) \tilde{\nu}_{j,\ell,x}(\mathrm{d}s') + h_j^{2\beta}$$

then:

(e1) if $\ell < L(j)$, then set $\lambda_{j,\ell+1} := \tilde{\lambda}_j$, $d_{j,\ell+1} := d_{j,\ell}/2$, $\varepsilon := d_{j,\ell}/2$, $\ell := \ell + 1$, and go to (b).

(e2) if $\ell = L(j)$, then set $u_j^{(k+1)} := \tilde{u}_j$, $\nu_{j,\ell}^{(k+1)} := \tilde{\nu}_{j,\ell}$, $\ell := 0$, and go to (g).

(f) Set $\varepsilon := 2\varepsilon$, $\lambda_{j,\ell} := \tilde{\lambda}_j$, and go to (c).

(g) If $\|u_j^{(k+1)} - u_j^{(k)}\|_{L^2(\Omega)} \leq h_j^2$ set $u_j := u_j^{(k+1)}$, $\nu_j := \tilde{\nu}_{j,\ell}^{(k+1)}$, $k := 0$, and go to (j).

(h) Set $k := k + 1$, $d_{j,\ell} := 2^{L(j)} h_j^\beta$, $\varepsilon := h_j/2$, $\lambda_{j,\ell} := \tilde{\lambda}_j$ and go to (b).

(j) Compute error indicators η_E for all sides $E \in \mathcal{E}(\mathcal{T}_j)$ in $\mathcal{T}_j$.

(k) Terminate if a stopping criterion is satisfied.

(l) Mark the side $E \in \mathcal{E}(\mathcal{T}_j)$ for refinement if $\eta_E \geq \Theta \max_{E' \in \mathcal{E}(\mathcal{T}_j)} \eta_{E'}$.

(m) Generate a new triangulation $\mathcal{T}_{j+1}$. Set $\lambda_{j+1,\ell} := \lambda_{j,L(j)}$, $u_{j+1}^{(k)} := u_j$, $\varepsilon := h_j$, $d_{j+1,\ell} := 2^{L(j+1)} h_{j+1}^\beta$, $j := j + 1$, and go to (b).

Remark 6.3.

(i) A computable criterion is available to enlarge m in (e) and thereby guarantee that it is large enough [4].

(ii) Feasibility of $(\mathfrak{RP}^{(k+1)}_{d_j,\ell,h_j,A})$ in Step (c) of the algorithm can be achieved, e.g., by enlarging A such that $\delta_{\nabla u_j^{(k)}} \in \mathcal{Y}_{d_j,\ell,h_j,A}(\Omega;\mathbb{R}^2)$.

(iii) Stopping criteria in (k) of Algorithm $(\mathcal{A}_{\mathcal{T}_0,\Theta,\beta,L,m})$ can be, e.g., $\|u_j - u_{j-1}\|_{L^2(\Omega)} \leq \varepsilon_{\text{stop}}$, $\|\lambda_j - \lambda_{j-1}\|_{L^{p'}(\Omega)} \leq \varepsilon_{\text{stop}}$, or $\sum_{E\in\mathcal{E}(\mathcal{T}_j)} \eta_E^{p'} \leq \varepsilon_{\text{stop}}$ for some $\varepsilon_{\text{stop}} > 0$, or $j = J$ for some $J \geq 1$.

(iv) Since in the optimal case we have $\|u_j - u\|_{L^2(\Omega)} \leq Ch_j^2$ we chose $\varepsilon_{\text{FP}} = h_j^2$ as a stopping criterion for the fixed point iteration.

(v) The tolerance $h_j^{2\beta}$ for the verification of the maximum principle in (e) guarantees $\lambda_j(x) = [F^{**}]'_s(x, \nabla u_j(x)) + \mathcal{O}(h_j^\beta)$ for almost all $x \in \Omega$.

(vi) The choices of ε for the definition of A in (c) are motivated by Proposition 5.1.

(vii) We refer to [47] for details on red-green-blue refinement strategies to obtain a refined regular triangulation from the error indicators η_E in (m).

(viii) Steps (b)-(e) of the algorithm realize the active set strategy as proposed in [13].

(ix) Since optimization toolboxes provide a Lagrange multiplier $\tilde{\lambda}$ based on duality (and hence the inner product in) $\mathbb{R}^N$, $\tilde{\lambda}$ has to be rescaled by $1/|T|$, i.e., $\lambda^{(k)}_{d,h}|_T := \tilde{\lambda}|_T/|T|$, in order to satisfy the conditions of Lemma 4.1.

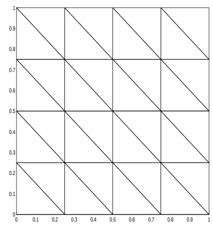

FIGURE 1. Initial triangulation $\mathcal{T}_0$ in the example.

For the numerical approximation of $(\mathfrak{RP})$ specified through (6.1)-(6.3) we choose a coarse initial triangulation $\mathcal{T}_0$ of Ω which consists of 32 congruent triangles with $N_0 = 25$ nodes, cf. Figure 1. We used $m = 2$, employed $L = (4, 2, 2, 2, ...)$, and tried all combinations of $\beta \in \{1, 3/2, 2\}$ and $\Theta \in \{0, 1/2\}$. Moreover, we used $\lambda_{0,0} = 0$ and $u_0^{(0)} = \mathcal{I}_{\mathcal{T}_0} u_{\text{D}}$ in Step (a) of the algorithm to start the iteration. As a stopping criterion we used $j = J$ for various positive integers J.

Figure 2 shows the solution $u_2 \in V_{h_2}(\Omega)$ on the uniform triangulation $\mathcal{T}_2$ for $\beta = 1$ and the support of the discrete Young measure solution restricted to two different elements. The triangulation $\mathcal{T}_2$ is obtained by two red-refinements of $\mathcal{T}_0$ and consists of 256 elements and has 225 free nodes. The displayed triangulation of $\omega = (-2, 2)^2$ admits 4761 nodes and we observe that the active set strategy activates only a few nodes (or atoms) which are very close to the support of the exact Young measure solution. In the middle plot of Figure 2 we observe some active nodes close to zero which results from Step (c) of the algorithm to ensure feasibility of the optimization problem $(\mathfrak{RP}^{(k+1)}_{d_j,\ell,h_j,A})$.

For a comparison we displayed the solution $u_{12} \in V_{h_{12}}(\Omega)$ on the adaptively generated triangulation $\mathcal{T}_{12}$ for $\beta = 3/2$ together with the support of the associated Young measure solution restricted to two different elements in Figure 3. The triangulation $\mathcal{T}_{12}$ admits a comparable number of degrees of freedom as the one shown

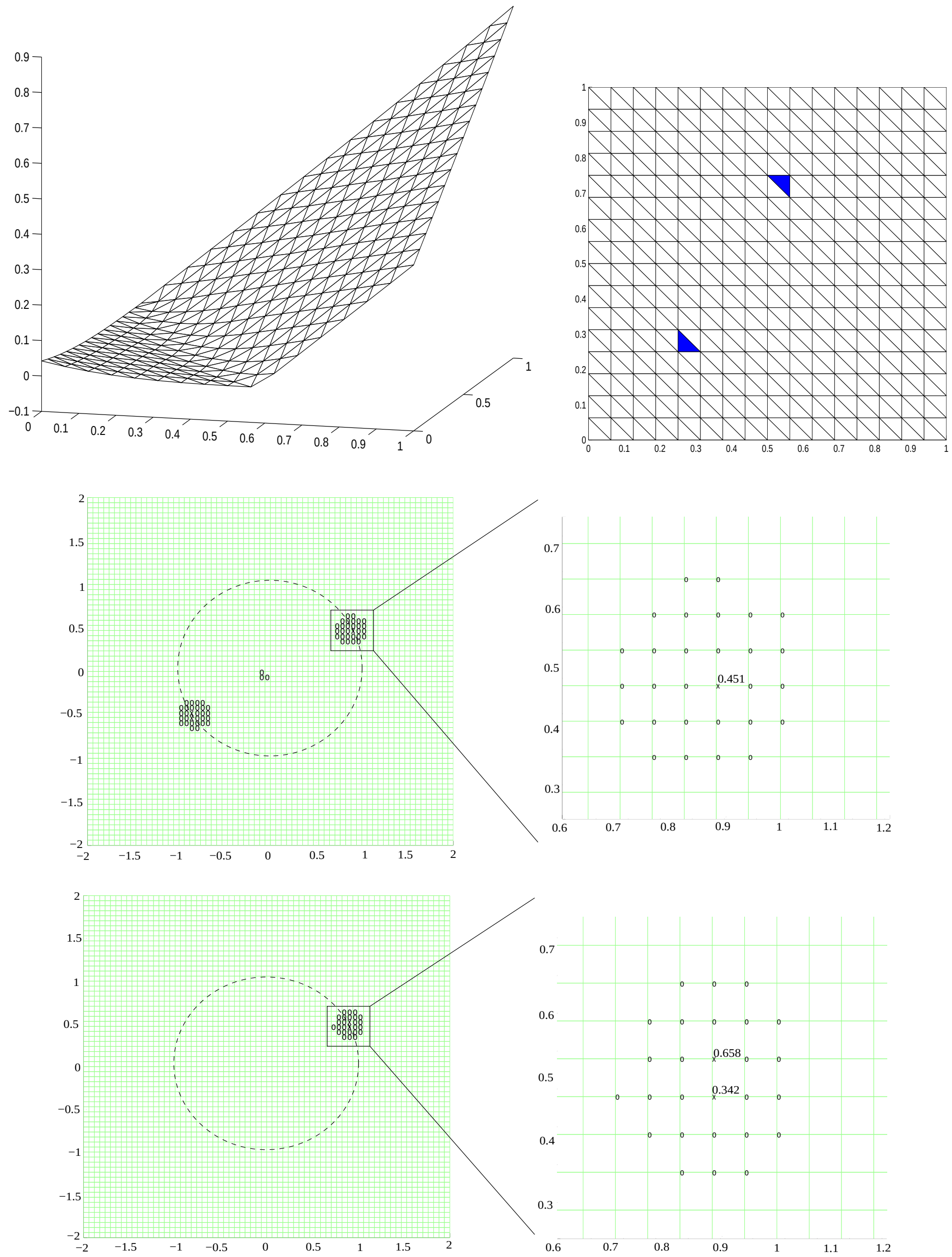

FIGURE 2. Solution on a uniformly refined triangulation (top) for $\beta = 1$ and support of the associated discrete Young measure (indicated by circles) restricted to the elements $\mathrm{conv}\{(5,4),(4,5),(4,4)\}/16$ (middle) and $\mathrm{conv}\{(8,12),(9,11),(9,12)\}/16$ (bottom) (indicated by a darker shading in the upper right plot). The magnified regions display volume fractions larger than $1/1000$.

in Figure 2 but the mesh on ω is finer because of the different choice of β. The adaptive refinement strategy refines the mesh towards the line $\{x \in \Omega; x \cdot a = \xi_b\}$ along which the exact solution has a discontinuity in the gradient. This appears reasonable since by our choice of ϕ uniform triangulations do not resolve that line and the approximation error in a neighbourhood of it is expected to be large on uniform meshes.

Table 1 displays for $\Theta = 0$, i.e., for uniform mesh refinement, $\beta = 1$, and $j = 0,1,2$ the number of free nodes in $\mathcal{T}_j$, the minimal integer K for which $\|u_j^{(K+1)} - u_j^{(K)}\|_{L^2(\Omega)} \le h_j^2$, the number of iterations in the active set strategy in the last step of the fixed point iteration and for the highest level $L(j)$ in the active set strategy, the number of atoms in the triangulation $\tau_{j,L(j)}$, as well as the average number

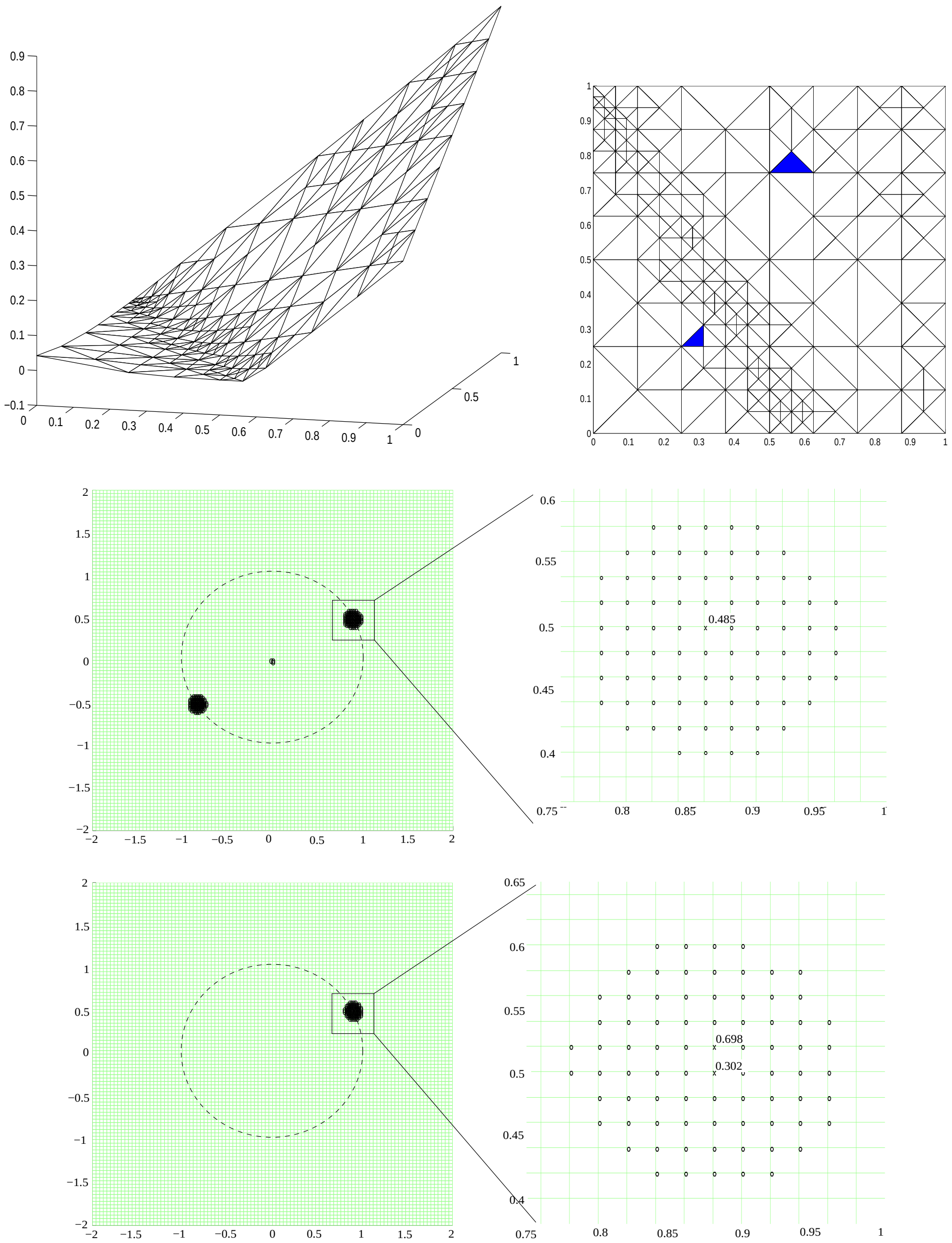

FIGURE 3. Solution on an adaptively refined triangulation (top) for $\beta = 3/2$ and support of the associated discrete Young measure (indicated by circles) restricted to the elements $\mathrm{conv}\{(5,5),(4,4),(5,4)\}/16$ (middle) and $\mathrm{conv}\{(10,12),(8,12),(9,13)\}/16$ (bottom) (indicated by a darker shading in the upper right plot). The magnified regions display volume fractions larger than $1/1000$.

of active atoms per element. It is remarkable that less than 4% of the possible atoms are activated by Algorithm $(\mathcal{A}_{\mathcal{T}_0,\Theta,\beta,L,m})$. Because of the nested iteration, i.e., choosing the solution on a coarse triangulation as the starting value for the fixed point iteration on the refined triangulation, the algorithm performs very few iterations for the fixed point iteration on one triangulation $\mathcal{T}_j$. The number of iterations in the maximum principle grows rapidly in this example. This behaviour might be caused by the choice of the parameter $\varepsilon = h_j$ (motivated by the estimate $\|\lambda_{j+1} - \lambda_j\|_{L^{4/3}(\Omega;\mathbb{R}^2)} \le C h_j$ which holds if the exact solution of $(\mathfrak{RP})$ is smooth) which seems too optimistic in this example.

The same numbers are displayed for $\Theta = 1/2$, i.e., adaptive mesh-refinement, and $\beta = 3/2$ in Table 2. Owing to the larger choice of β the number of possible atoms grows faster but less than 3% of them are activated by the active set strategy. Again, the number of fixed point iterations is very small but in contrast to the numbers for uniform mesh refinement, the numbers of iterations in the maximum principle seem to remain bounded.

j	dof($\mathcal{T}_j$)	FP-it's	MP-it's	# atoms/$\lvert\mathcal{T}_j\rvert$	# active atoms/$\lvert\mathcal{T}_j\rvert$
0	9	3	1	289	9.3
1	49	3	12	1369	21.3
2	225	3	30	4761	65.1

TABLE 1. Degrees of freedom (=dof) in $\mathcal{T}_j$, numbers of fixed point (FP-) and maximum principle (MP-) iterations, numbers of possible atoms, and average number of activated atoms per element in the final iteration on $\mathcal{T}_j$ for uniform mesh refinement and $\beta = 1$.

j	dof($\mathcal{T}_j$)	FP-it's	MP-it's	# atoms/$\lvert\mathcal{T}_j\rvert$	# active atoms/$\lvert\mathcal{T}_j\rvert$
0	9	3	2	1089	17.8
1	12	3	2	2401	32.2
2	20	3	2	3721	44.2
3	34	3	1	5929	48.3
4	37	3	1	6561	55.3
5	52	3	3	9409	71.5
6	59	3	4	11025	73.6
7	70	3	7	13689	85.4
8	83	3	2	17689	93.9
9	121	3	6	29929	120.5
10	146	3	3	37249	122.6
11	147	3	2	38809	131.6
12	152	3	6	40401	131.6

TABLE 2. Degrees of freedom (=dof) in $\mathcal{T}_j$, numbers of fixed point (FP-) and maximum principle (MP-) iterations, numbers of possible atoms, and average number of activated atoms per element in the final iteration on $\mathcal{T}_j$ for adaptive mesh refinement and $\beta = 3/2$.

For all combinations of $\Theta \in \{0, 1/2\}$ and $\beta \in \{1, 3/2, 2\}$ we displayed the error $\|u_j - u\|_{L^2(\Omega)}$ against degrees of freedom in $\mathcal{T}_j$ for $j = 0, 1, 2, ...$ with a logarithmic scaling used for both axes in Figure 4. We observe that the adaptive refinement strategy for $\beta = 3/2$ leads to smaller errors than the uniform refinement strategy for $\beta = 3/2$ at comparable numbers of degrees of freedom in $\mathcal{T}_j$ larger than 100, and also to an improved experimental convergence rate. For the theoretically motivated choice $\beta = 2$ we were not able to compute solutions on meshes with more than 100 degrees of freedom in $\mathcal{T}_j$. The numerical results indicate however that the choice $\beta = 2$ is too pessimistic in this example and $\beta = 1$ appears sufficient for uniform mesh-refinement. For the adaptive strategy the choice $\beta = 1$ gave suboptimal results but $\beta = 3/2$ led to reasonable solutions.

For all combinations of $\Theta \in \{0, 1/2\}$ and $\beta \in \{1, 3/2, 2\}$ in Algorithm $(\mathcal{A}_{\mathcal{T}_0,\Theta,\beta,L,m})$ Figure 5 displays the error $\|\lambda_j - \lambda\|_{L^{4/3}(\Omega;\mathbb{R}^2)}$ for $\lambda = [F^{**}]'_s(\cdot, \nabla u)$ on various triangulations. We observe that the stress error decreases optimally with rate 1/2 for

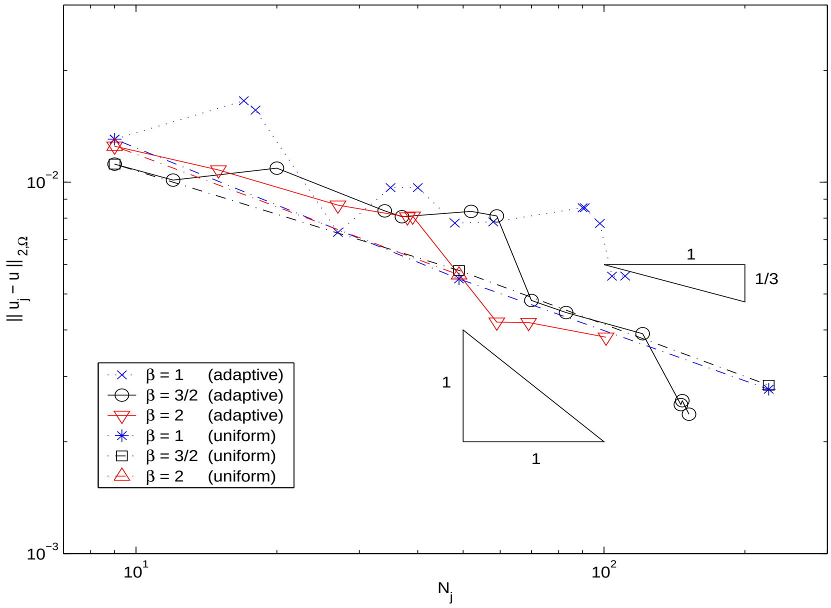

FIGURE 4. L^2 error for all combinations of $\Theta \in \{0, 1/2\}$ and $\beta \in \{1, 3/2, 2\}$ in Algorithm $(\mathcal{A}_{\mathcal{T}_0,\Theta,\beta,L,m})$.

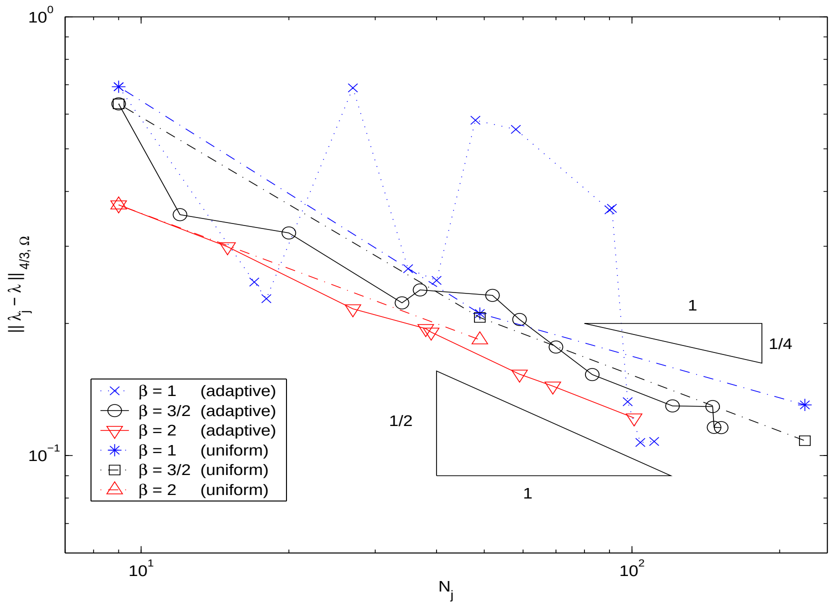

FIGURE 5. Stress error for uniform and adaptive mesh refinement and $\beta = 1, 3/2, 2$.

$(\Theta, \beta) = (1/2, 3/2)$. The plot also shows that the choice $\beta = 1$ is not sufficient for adaptive mesh refinement. The stress error for $(\Theta, \beta) = (0, 3/2)$ is smaller than the error for $(\Theta, \beta) = (0, 1)$ so that the choice $\beta = 1$ might lead to suboptimal results for the stress error in this example.

In Figure 6 we displayed the stress error together with the error estimators $\eta_{R,R}$, $\eta_{R,E}$, $\eta_{A,R}$, and $\eta_{A,E}$ for $(\Theta, \beta) = (0, 1), (1/2, 3/2)$. The stress error seems to decay faster (with optimal experimental convergence rate $1/2$) for adaptive mesh refinement and $\beta = 3/2$, while the plot indicates a suboptimal experimental convergence rate $1/6$ for uniform refinement and $\beta = 1$. The error estimator $\eta_{A,E}$ serves as a good approximation of the stress error in contrast to $\eta_{A,R}$ and $\eta_{R,R}$ which converge slower and have to be regarded as reliable upper bounds. To make a final conclusion about the performance of the error estimators one would however have to use finer meshes as we may may still be in the preasymptotic range for $\mathrm{dof}(\mathcal{T}_j) \leq 250$.

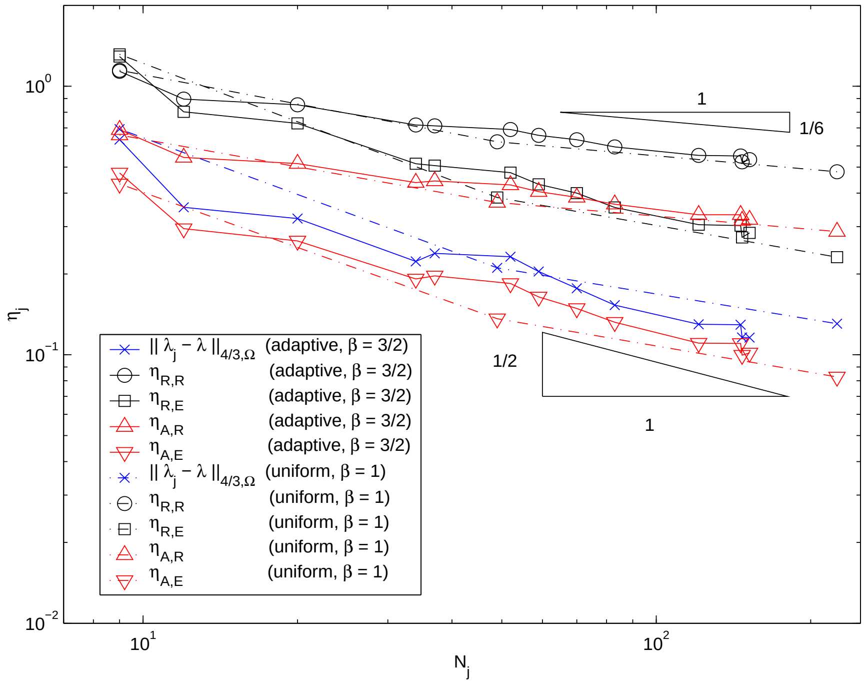

FIGURE 6. Stress error and error estimators for $(\Theta, \beta) = (0, 1)$ and $(\Theta, \beta) = (1/2, 3/2)$ in Algorithm $(\mathcal{A}_{\mathcal{T}_0,\Theta,\beta,L,m})$.

7. Further examples

The scalar character of the addressed variational problems as well as the assumption (3.1) restricts application area of our approach considerably. Hence it is worth outlining applicability of our algorithm to three specific models having definite interpretations.

7.1. Compatible phase transitions in elastic solids.

This first example is out of the scalar framework used throughout this paper and illustrates how the applications of the algorithm can be widened to vectorial problems at least in special cases. Given two symmetric matrices $E_1, E_2 \in \mathbb{R}^{n\times n}_{\mathrm{sym}}$ such that $E_2 - E_1 = (a \otimes b + b \otimes a)/2$ for $a, b \in \mathbb{R}^n$ with $|b| = 1$, and a symmetric, positive-definite fourth order tensor $\mathbb{C}$, the function

$$F(x, E) = F(E) := \frac{1}{2} \min_{j=1,2} |\mathbb{C}^{1/2}(E - E_j)|^2, \qquad E \in \mathbb{R}^{n\times n}_{\mathrm{sym}} \tag{7.1}$$

leads to a simple model for compatible phase transitions in certain elastic solids at small strains provided, of course, $(\mathfrak{P})$ employs $W^{1,p}(\Omega;\mathbb{R}^n)$ instead of $W^{1,p}(\Omega)$, appropriate functions G and u_D, and the symmetric gradient $\varepsilon(u) := \frac{1}{2}(\nabla u + \nabla u^T)$ instead of ∇u. We refer to [1, 12] for specifications of E_1, E_2 and $\mathbb{C}$ that model a tetragonal-to-monoclinic transformation in a high-temperature superconductor. Owing to the work of [26] and the choice of E_1, E_2, formulation $(\mathfrak{RP})$ (with $\mathbb{R}^n$ replaced by $\mathbb{R}^{n\times n}_{\mathrm{sym}}$) is a proper relaxation of $(\mathfrak{P})$. The following lemma shows that the key assumptions (3.1) and (4.7) of our analysis are indeed satisfied in this example.

Lemma 7.1. *Let F be defined through (7.1). Then F^{**} satisfies (3.1) and (4.7).*

Proof. It is shown in [5] that $F^{**}(E) = \frac{1}{2}\min_{\theta\in[0,1]} |\mathbb{C}^{1/2}(E - (1-\theta)E_1 - \theta E_2)|^2 = \frac{1}{2}\min_{\theta\in[0,1]} |\mathbb{C}^{1/2}(E - E_1 - \theta A)|^2$ where $A := (a\otimes b + b\otimes a)/2$. If $\theta(E) \in [0,1]$ satisfies $F^{**}(E) = \frac{1}{2}|\mathbb{C}^{1/2}(E - E_1 - \theta(E)A)|^2$ then (with ":" denoting the scalar product in

$\mathbb{R}^{n\times n}$)

$$\frac{1}{|\mathbb{C}^{1/2}A|^2}\mathbb{C}(E-E_1):A\begin{cases}\le 0, & \text{for } \theta(E)=0,\\ =\theta(E), & \text{for } \theta(E)\in(0,1),\\ \ge 1, & \text{for } \theta(E)=1.\end{cases} \tag{7.2}$$

According to [3] there holds $F^{**}\in C^1(\mathbb{R}^{n\times n}_{\text{sym}})$ and this implies that [5]

$$[F^{**}]'(E)=\mathbb{C}(E-E_1-\theta(E)A).$$

Given $E,\tilde{E}\in\mathbb{R}^{n\times n}_{\text{sym}}$ let $\alpha\in\mathbb{R}$ and $A^\perp\in\mathbb{R}^{n\times n}_{\text{sym}}$ satisfy $\mathbb{C}A^\perp:A=0$ and $E-\tilde{E}=\alpha A+A^\perp$. Writing $\theta:=\theta(E)$ and $\tilde{\theta}:=\theta(\tilde{E})$ we have

$$\begin{aligned}([F^{**}]'(E)-[F^{**}]'(\tilde{E})):(E-\tilde{E})&=\mathbb{C}\big(\alpha A+A^\perp-(\theta-\tilde{\theta})A\big):\big(\alpha A+A^\perp\big)\\ &=\big(\alpha^2-\alpha(\theta-\tilde{\theta})\big)|\mathbb{C}^{1/2}A|^2+|\mathbb{C}^{1/2}A^\perp|^2.\end{aligned}$$

Since $\alpha=\frac{1}{|\mathbb{C}^{1/2}A|^2}\mathbb{C}(E-\tilde{E}):A$, the estimates in (7.2) allow for $\alpha^2-\alpha(\theta-\tilde{\theta})\ge 0$. This proves (3.1) since $A^\perp$ is the projection of E_1-E_2 onto the orthogonal complement of A. The identity

$$\begin{aligned}&([F^{**}]'(E)-[F^{**}]'(\tilde{E})):(E-\tilde{E})-|\mathbb{C}^{-1}([F^{**}]'(E)-[F^{**}]'(\tilde{E}))|^2\\ &\quad=\mathbb{C}\big(\alpha A+A^\perp-(\theta-\tilde{\theta})A\big):\big((\theta-\tilde{\theta})A\big)\\ &\quad=\alpha^2|\mathbb{C}^{1/2}A|^2-\alpha(\theta-\tilde{\theta})|\mathbb{C}^{1/2}A|^2\end{aligned}$$

leads to the proof of (4.7). □

Let us remark that extension to more than 2 wells is not simple at all, and has been done by Smyshlyaev and Willis [48] for a 3-well problem while only certain estimates are known for more than 3-wells [22].

7.2. **Optimal shape design problems.** Given $\Omega\subset\mathbb{R}^2$, a positive number $\alpha<|\Omega|$, and two positive numbers $\mu_1<\mu_2$ the following domain optimization problem models the optimal mixture of two materials and occurs in solid and fluid mechanics: *Find $u\in W^{1,2}(\Omega)$ and $\omega\subset\Omega$ such that $u|_{\partial\Omega}=0$, $|\omega|=a$, and the pair (u,ω) is minimal for*

$$I(u;\omega):=\int_\Omega \frac{1}{2}\mu(x)|\nabla u(x)|^2+u(x)\,\mathrm{d}x,$$

with $\mu|_\omega=\mu_1$ and $\mu|_{\Omega\setminus\omega}=\mu_2$. It has been shown in [21] that this problem can be reduced to the following saddle point problem: *Find $(\lambda,u)\in\mathbb{R}\times W^{1,2}(\Omega)$ with $u|_{\partial\Omega}=0$ which are optimal in*

$$\sup_{\lambda\in\mathbb{R}}\ \inf_{\substack{u\in W^{1,2}(\Omega)\\ u|_{\partial\Omega}=0}}\int_\Omega \Phi_\lambda(\nabla u(x))+u(x)\,\mathrm{d}x+C_0\lambda.$$

Here, Φ_λ is explicitly determined by λ (see [21, 11] for details) and μ_1,μ_2, is non-convex, and satisfies our assumptions (2.2), (2.3), and (4.7). Therefore, for each $\lambda\in\mathbb{R}$ we recover a scalar variational problem of the type $(\mathfrak{P})$ with $G(x,u)=u$. The assumption (3.1) is not satisfied but not needed for our approximation scheme because the resulting relaxed problem is linear and the algorithm converges always in one iteration. This situation is scrutinized in [4].

7.3. **Phase transitions in antiplane shear settings.** Nonlinear elasticity under very special circumstances leads to a so-called antiplane shear setting; cf. the survey paper by Horgan [24]. A multi-well stored energy then corresponds to various natural configurations of the material, called phases; cf. [20, 46] for this antiplane setting. For example, a two-dimensional double-well problem considered in [15, 20, 46] employs

$$F(x,s) = s_1^2 + as_2^4 - bs_2^2, \qquad a,b>0. \tag{7.3}$$

This $F(x,\cdot)$ allows for an explicit convex envelope

$$F^{**}(x,\cdot) = s_1^2 + \begin{cases} -b^2/(4a) & \text{if } s_2 \in \big[-\sqrt{b/(2a)}, \sqrt{b/(2a)}\big], \\ as_2^4 - bs_2^2 & \text{otherwise.} \end{cases} \tag{7.4}$$

Here F^{**} satisfies (3.1) with $s^* = (1,0)$ and $c_4 = 1$, but (3.3) would have to be naturally modified and an anisotropic Sobolev space would have to be used. As to the weighted uniform monotonicity (4.7) of an inverse to $[F^{**}]'_s(x,\cdot)$, it holds here in a suitable "anisotropic" modification with $\varrho = 2$ (resp. 4/3) and $\sigma = 1$ (resp. 3) with respect to s_1 (resp. s_2) because $|[F^{**}]'_s(x,\cdot)|$ has a growth as power $\sigma = 1$ (resp. 3) with respect to s_1 (resp. s_2).

A more general case considers k phases described by the gradients $\{s_i\}_{i=1}^k \subset \mathbb{R}^n$, positive-definite matrices $\{C_i\}_{i=1}^k \subset \mathbb{R}^{n\times n}_{\rm sym}$ of "elastic" moduli, offsets $\{w_i\}_{i=1}^k \subset \mathbb{R}$, and elastic response near the phases that can be described by the potential

$$F(x,s) = F(s) := \min_{i=1,\dots,k} \Big(\frac{1}{2}|C_i^{1/2}(s-s_i)|^2 + w_i\Big). \tag{7.5}$$

The following lemma describes the convex envelope of F and proves that all our assumptions are satisfied if $k \le n$ and $C_1 = \dots = C_k =: C$.

Lemma 7.2. *Let $F(x,s) = F(s)$ be as in (7.5) with $C_i = C \in \mathbb{R}^{n\times n}_{\rm sym}$ positive definite, $i = 1,2,\dots,k$.*
(i) For $s \in \mathbb{R}^n$ there holds

$$F^{**}(s) = \min_{\substack{\theta_i\in[0,1] \\ \theta_1+\dots+\theta_k=1}} \frac{1}{2}\Big|C^{1/2}\big(s - \sum_{i=1}^k \theta_i s_i\big)\Big|^2 + \sum_{i=1}^k \theta_i w_i. \tag{7.6}$$

(ii) If for $s \in \mathbb{R}^n$ the convex-combination coefficients θ_i, $i = 1,\dots,k$, are optimal in (7.6) then

$$[F^{**}]'(s) = C\big(s - \sum_{i=1}^k \theta_i s_i\big). \tag{7.7}$$

(iii) For $s, \tilde s \in \mathbb{R}^n$ there holds

$$\big|C^{-1}\big([F^{**}]'(s) - [F^{**}]'(\tilde s)\big)\big|^2 \le \big([F^{**}]'(s) - [F^{**}]'(\tilde s)\big)\cdot(s-\tilde s). \tag{7.8}$$

(iv) Let $L \subset \mathbb{R}^n$ be a linear subspace of $\mathbb{R}^n$ and $\ell_0 \in L^\perp$ (here orthogonality is defined through the scalar product $(s,\tilde s) \mapsto (Cs)\cdot\tilde s$) such that conv $\{s_1, s_2, \dots, s_k\} \subset \ell_0 + L$. *Let $\ell^\perp \in L^\perp$ such that $|C^{1/2}\ell^\perp| = 1$. For $s, \tilde s \in \mathbb{R}^n$ there holds*

$$\big(C\ell^\perp\cdot(s-\tilde s)\big)^2 \le \big([F^{**}]'(s) - [F^{**}]'(\tilde s)\big)\cdot(s-\tilde s).$$

Proof. (i) Formula (7.6) follows from showing that $F^{**}(s)$ is bounded from above by the right-hand side RHS(s) of (7.6), that RHS is a convex function, and that RHS(s) $\le F(s)$. The fact that F^{**} is the largest convex function below F yields (7.6).

(ii) For a proof of (7.7) let $s \in \mathbb{R}^n$ and θ_i, $i = 1, ..., k$, be optimal for s in (7.6), and let us abbreviate $(s_\theta, w_\theta) = \sum_{i=1}^k \theta_i(s_i, w_i)$. For any $s' \in \mathbb{R}^n$ and $t \in \mathbb{R}$ we have

$$F^{**}(s + ts') \le \frac{1}{2}|C^{1/2}(s + ts' - s_\theta)|^2 + w_\theta.$$

Hence, there holds

$$\begin{aligned} F^{**}(s + ts') - F^{**}(s) &\le \frac{1}{2}|C^{1/2}(s + ts' - s_\theta)|^2 - \frac{1}{2}|C^{1/2}(s - s_\theta)|^2 \\ &= \frac{1}{2}C(s + ts' - s_\theta) \cdot (s + ts' - s_\theta) - \frac{1}{2}C(s - s_\theta) \cdot (s - s_\theta) \\ &= C(s - s_\theta) \cdot (ts') + \frac{1}{2}t^2|C^{1/2}s'|^2. \end{aligned}$$

Since we know from [3] that $F^{**} \in C^1(\mathbb{R}^n)$ we have, for $|t| \le t_0$,

$$F^{**}(s + ts') = F^{**}(s) + t[F^{**}]'(s) \cdot s' + \varphi(t)$$

with $\varphi(t)/|t| \to 0$ for $t \to 0$. Hence, for all $|t| \le t_0$ there holds

$$\frac{t}{|t|}\big([F^{**}]'(s) - C(s - s_\theta)\big) \cdot s' \le \frac{-\varphi(t)}{|t|} + \frac{|t|}{2}\,|C^{1/2}s'|^2$$

and this implies (by choosing an appropriate sign for $t \to 0$)

$$\big(C(s - s_\theta) - [F^{**}]'(s)\big) \cdot s' = 0.$$

Since $s' \in \mathbb{R}^n$ was arbitrary we deduce $[F^{**}]'(s) = C(s - s_\theta)$.

(iii) Given any $s, \tilde{s} \in \mathbb{R}^n$, let $\theta_i, \varrho_i \in [0, 1]$, $i = 1, ..., k$ be such that $\sum_{i=1}^k \theta_i = \sum_{i=1}^k \varrho_i = 1$ and

$$F^{**}(s) = \frac{1}{2}|C^{1/2}(s - s_\theta)|^2 + w_\theta \quad \text{and} \quad F^{**}(\tilde{s}) = \frac{1}{2}|C^{1/2}(\tilde{s} - \tilde{s}_\varrho)|^2 + \tilde{w}_\varrho$$

where $(s_\theta, w_\theta) = \sum_{i=1}^k \theta_i(s_i, w_i)$ and $(\tilde{s}_\varrho, \tilde{w}_\varrho) = \sum_{i=1}^i \varrho_i(s_i, w_i)$. (7.7) shows

$$\big|C^{-1}\big([F^{**}]'(s) - [F^{**}]'(\tilde{s})\big)\big|^2 = C(s - s_\theta - \tilde{s} + \tilde{s}_\varrho) \cdot (s - s_\theta - \tilde{s} + \tilde{s}_\varrho)$$

and

$$\big([F^{**}]'(s) - [F^{**}]'(\tilde{s})\big) \cdot (s - \tilde{s}) = C(s - s_\theta - \tilde{s} + \tilde{s}_\varrho) \cdot (s - \tilde{s}).$$

Using $\sum_{i=1}^k \varrho_i = \sum_{i=1}^k \theta_i = 1$ we find

$$\begin{aligned} &\big([F^{**}]'(s) - [F^{**}]'(\tilde{s})\big) \cdot (s - \tilde{s}) - |C^{-1}([F^{**}]'(s) - [F^{**}]'(\tilde{s}))|^2 \\ &\quad = C(s - s_\theta - \tilde{s} + \tilde{s}_\varrho) \cdot (s_\theta - \tilde{s}_\varrho) \\ &\quad = C(s - s_\theta) \cdot (s_\theta - \tilde{s}_\varrho) - C(\tilde{s} - \tilde{s}_\varrho) \cdot (s_\theta - \tilde{s}_\varrho) \\ &\quad = \sum_{\ell=1}^k \varrho_\ell C(s - s_\theta) \cdot (s_\theta - s_\ell) + \sum_{\ell=1}^k \theta_\ell C(\tilde{s} - \tilde{s}_\varrho) \cdot (\tilde{s}_\varrho - s_\ell) \\ &\quad = \sum_{\ell=1}^k \varrho_\ell\Big(C(s - s_\theta) \cdot (s_\theta - s_\ell) - w_\theta + w_\ell\Big) \\ &\qquad + \sum_{\ell=1}^k \theta_\ell\Big(C(\tilde{s} - \tilde{s}_\varrho) \cdot (\tilde{s}_\varrho - s_\ell) - \tilde{w}_\varrho + w_\ell\Big). \end{aligned} \tag{7.9}$$

By choice of θ_i, $i = 1, ..., k$, for each $\ell \in \{1, ..., k\}$ the mapping $f_\ell : [0, 1] \to \mathbb{R}$,

$$\alpha \mapsto |C^{1/2}(s - \alpha s_\theta - (1 - \alpha)s_\ell)|^2/2 + \alpha w_\theta + (1 - \alpha)w_\ell$$

has a minimum in $\alpha = 1$, i.e., $f'_\ell(1) \le 0$, or

$$-C(s - s_\theta) \cdot (s_\theta - s_\ell) + w_\theta - w_\ell \le 0.$$

The same argument shows for all $\ell \in \{1, ..., N\}$,

$$-C(\tilde{s} - \tilde{s}_\varrho) \cdot (\tilde{s}_\varrho - s_\ell) + \tilde{w}_\varrho - w_\ell \le 0.$$

Hence, the right-hand side of (7.9) is non-negative and this implies (iii).

(iv) Let $s_L, \tilde{s}_L \in L$ and $s^\perp, \tilde{s}^\perp \in L^\perp$ such that, with respect to the scalar product $\langle x, y\rangle_C := (Cx) \cdot y$, we have the orthogonal decompositions

$$s - \ell_0 = s_L + s^\perp \quad \text{and} \quad \tilde{s} - \ell_0 = \tilde{s}_L + \tilde{s}^\perp.$$

Let $\theta_i, \varrho_i \in [0,1]$ and (s_θ, w_θ), $(\tilde{s}_\varrho, \tilde{w}_\varrho)$ be as in the proof of (iii). Using repeatedly orthogonality of elements in L and $L^\perp$ we verify

$$\begin{aligned}
&\big([F^{**}]'(s) - [F^{**}]'(\tilde{s})\big) \cdot (s - \tilde{s}) - |C^{1/2}(s^\perp - \tilde{s}^\perp)|^2 \\
&\qquad = \langle s - s_\theta - \tilde{s} + \tilde{s}_\varrho, s - \tilde{s}\rangle_C - \langle s^\perp - \tilde{s}^\perp, s^\perp - \tilde{s}^\perp\rangle_C \\
&\qquad = \langle s - s_\theta - \tilde{s} + \tilde{s}_\varrho, s - \tilde{s}\rangle_C - \langle s^\perp - \tilde{s}^\perp, s - \tilde{s}\rangle_C \\
&\qquad = \langle s_L - s_\theta - \tilde{s}_L + \tilde{s}_\varrho, s - \tilde{s}\rangle_C \\
&\qquad = \langle s_L - s_\theta - \tilde{s}_L + \tilde{s}_\varrho, s_\theta - \tilde{s}_\varrho\rangle_C + \langle s_L - s_\theta - \tilde{s}_L + \tilde{s}_\varrho, s - s_\theta - \tilde{s} + \tilde{s}_\varrho\rangle_C \\
&\qquad = \langle s_L - s_\theta - \tilde{s}_L + \tilde{s}_\varrho, s_\theta - \tilde{s}_\varrho\rangle_C + \langle s_L - s_\theta - \tilde{s}_L + \tilde{s}_\varrho, s_L - s_\theta - \tilde{s}_L + \tilde{s}_\varrho\rangle_C \\
&\qquad = \langle s_L - s_\theta - \tilde{s}_L + \tilde{s}_\varrho, s_\theta - \tilde{s}_\varrho\rangle_C + \left|C^{1/2}(s_L - s_\theta - \tilde{s}_L + \tilde{s}_\varrho)\right|^2 \\
&\qquad \ge \langle s_L - s_\theta - \tilde{s}_L + \tilde{s}_\varrho, s_\theta - \tilde{s}_\varrho\rangle_C \\
&\qquad = \langle s - s_\theta - \tilde{s} + \tilde{s}_\varrho, s_\theta - \tilde{s}_\varrho\rangle_C.
\end{aligned}$$

This right-hand side equals the right-hand side of (7.9) which has been shown to be non-negative in the proof of (iii). □

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