Adaptive Multilevel – Methods for Obstacle Problems in Three Space Dimensions

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Abstract. We consider the discretization of obstacle problems for second order elliptic differential operators in three space dimensions by piecewise linear finite elements. Linearizing the discrete problems by suitable active set strategies, the resulting linear sub-problems are solved iteratively by preconditioned cg-iterations. We propose a variant of the BPX preconditioner and prove an O(j) estimate for the resulting condition number. To allow for local mesh refinement we derive semi-local and local a posteriori error estimates. The theoretical results are illustrated by numerical computations.

Key words: obstacle problems, adaptive finite element methods, multilevel preconditioning, a posteriori error estimates

AMS (MOS) subject classifications: 65N30, 65N50, 65N55, 35J85, 49J40

Chapter 1

Introduction

Given a closed subspace $V \subset H^1(\Omega)$, Ω being a bounded polyhedral domain in the Euclidean space \mathbb{R}^3 , we consider obstacle problems of the form

Find $u \in K$ such that $\mathcal{J}(u) \leq \mathcal{J}(v), v \in K$, (1.1)

for the energy functional \mathcal{J} ,

$$\mathcal{J}(v) = \frac{1}{2}a(v,v) - \ell(v) , \quad v \in V,$$

and a closed, convex set $K \subset V$,

$$K = \{ v \in V | v(\mathbf{x}) \le \varphi(\mathbf{x}) \text{ a.e. in } \Omega \}.$$

Assuming that \mathcal{J} is induced by a symmetric V-elliptic bilinear form $a(\cdot, \cdot)$,

$$a(v,w) = \int_{\Omega} \sum_{i,j=1}^{3} a_{ij} \,\partial_i v \,\partial_j w \,d\mathbf{x},$$

and some functional $\ell \in V'$, it is well-known that (1.1) is equivalent to the variational inequality

Find
$$u \in K$$
 such that $a(u, u - v) \le \ell(u - v)$, $v \in K$. (1.2)

For simplicity we restrict our considerations to the case $V = H_0^1(\Omega)$. To ensure existence and uniqueness of the solution u of (1.1) and (1.2), respectively, we assume $\varphi \in H^1(\Omega), \varphi \geq 0$ a.e. on the boundary $\partial\Omega$, and $a_{ij} \in L^{\infty}(\Omega)$ satisfying

a)
$$a_{ij}(\mathbf{x}) = a_{ji}(\mathbf{x}), \ 1 \le i, \ j \le 3,$$

b) $\alpha_0 |\xi|^2 \le \sum_{i,j=1}^3 a_{ij}(\mathbf{x}) \xi_i \xi_j \le \alpha_1 |\xi|^2, \ \xi \in \mathbb{R}^3, \ 0 < \alpha_0 \le \alpha_1.$
(1.3)

for almost all $\mathbf{x} \in \Omega$.

Discretizing (1.2) in space by continuous, piecewise linear finite elements with respect to a partition \mathcal{T} of Ω in tetrahedra, we consider the efficient solution of the resulting finite dimensional variational inequality together with the appropriate choice of \mathcal{T} .

As the convergence rate of standard projected relaxation methods (e.g. [16]) is well-known to deteriorate with increasing refinement, a variety of multigrid

methods has been developed in the last decade. For an overview we refer to [23]. In the present paper we consider some sort of linearization based on active set strategies (e.g. [18, 19, 20]). This is a class of iterative schemes where in each iteration step a set of active constraints is prespecified and then a reduced linear sub-problem has to be solved for the computation of the new iterate. In the following section we will briefly recall the algorithm proposed in [19, 20].

The reduced linear problems arising in each step of the active set strategy can be regarded as usual Dirichlet problems on some reduced computational domain and hence may be solved iteratively by appropriate multigrid methods [18, 19, 20] or multilevel preconditioned cg-iterations [22, 23]. The construction and analysis of a suitable variant of the BPX preconditioner [10] will be subject of Section 3. Using the well-known interpretation as additive Schwarz methods [7, 34, 37, 38], it is shown that the condition number is bounded in terms of O(j) provided that the free boundary is sufficiently regular. Note that the regularity condition is resulting from the non-local character of the L^2 -projection compared to the interpolation arising in the analysis of the hierarchical basis preconditioner [23]. Probably, this non-optimal bound can be improved by more sophisticated techniques [9, 12, 31].

For the adaptive construction of a suitable hierarchy of triangulations, efficient and reliable a posteriori error estimates are required. In [23, 26] the basic concept of [13, 28] relying on suitable localizations of the discretized defect problem has been extended to variational inequalities. Related results in three space dimensions are presented in Section 4. Note that a posteriori estimates for a penalty method have been proposed in [25], while a recent generalization of the well–known Bank/Weiser estimator [4] can be found in [1].

The final section is devoted to some numerical experiments supporting the theoretical findings.

Chapter 2

Active Set Strategies

A partition \mathcal{T} of the computational domain $\Omega \subset \mathbb{R}^3$ in tetrahedra is called triangulation. Henceforth we only consider triangulations which are conforming in the sense that the intersection of two different tetrahedra $t, t' \in \mathcal{T}$ either consists of a common triangular face, a common edge, a common vertex or is empty. The sets of vertices p and edges e which are not part of the boundary $\partial\Omega$ are called \mathcal{N} and \mathcal{E} , respectively. We approximate $H^1_0(\Omega)$ by the subspace \mathcal{S} of continuous, piecewise linear finite elements vanishing on the boundary $\partial\Omega$. The nodal basis functions $\lambda_p \in \mathcal{S}, p \in \mathcal{N}$ are defined by $\lambda_p(q) = \delta_{pq}, p, q \in \mathcal{N}$, (Kronecker delta).

Further, let $\varphi_{\mathcal{T}} \in \mathcal{S}$ be a discrete obstacle approximating the given obstacle φ in an appropriate sense. For example, $\varphi_{\mathcal{T}}$ may be chosen as the L^2 -projection of φ onto \mathcal{S} or, if $\varphi \in C(\overline{\Omega})$, as the \mathcal{S} -interpolate. Correspondingly, we denote by $K_{\mathcal{T}} = \{v \in \mathcal{S} | v \leq \varphi_{\mathcal{T}}\}$ the set of discrete constraints. Then the finite element approximation of (1.1) amounts to the computation of an element $u_{\mathcal{T}} \in K_{\mathcal{T}}$ satisfying

$$a(u_{\mathcal{T}}, u_{\mathcal{T}} - v) \le \ell(u_{\mathcal{T}} - v), \ v \in K_{\mathcal{T}} .$$

$$(2.1)$$

The finite dimensional variational inequality (2.1) will be solved iteratively by the active set strategy proposed in [19, 20]:

Active set strategy

Step 1: Choose an initial iterate $u^{(0)} \in \mathcal{S}$.

Step 2: Given $u^{(\nu)} \in \mathcal{S}, \nu \geq 0$, determine the subset of active nodes $\mathcal{N}^{\bullet} \subset \mathcal{N}$ as the set of points $p \in \mathcal{N}$ such that

$$\varphi_{\mathcal{T}}(p) - u^{(\nu)}(p) \le \ell(\lambda_p) - a(u^{(\nu)}, \lambda_p)$$

while the remaining nodes $\mathcal{N}^{\circ} = \mathcal{N} \setminus \mathcal{N}^{\bullet}$ are called inactive. Introducing a direct splitting of the finite element space \mathcal{S} into the linear subspaces \mathcal{S}° , $\mathcal{S}^{\bullet} \subset \mathcal{S}$ defined by

$$\mathcal{S}^{\circ} = \{ v \in \mathcal{S} | v(p) = 0, p \in \mathcal{N}^{\bullet} \}, \ \mathcal{S}^{\bullet} = \{ v \in \mathcal{S} | v(p) = 0, p \in \mathcal{N}^{\circ} \}$$

the new iterate $u^{(\nu+1)} \in \mathcal{S}$ is computed from

$$u^{(\nu+1)} = u^{\bullet} + u^{\circ}, \qquad (2.2)$$

where $u^{\bullet} \in \mathcal{S}^{\bullet}$ is given by

$$u^{\bullet}(p) = \varphi_{\mathcal{T}}(p), \quad p \in \mathcal{N}^{\bullet},$$
 (2.3)

and $u^{\circ} \in \mathcal{S}^{\circ}$ is the solution of the reduced linear system

$$a(u^{\circ}, v) = \ell(v) - a(u^{\bullet}, v), \quad v \in \mathcal{S}^{\circ}.$$
(2.4)

Note that the reduced system (2.4) may be regarded as a Dirichlet problem on the reduced computational domain Ω° ,

$$\Omega^{\circ} = \bigcup_{p \in \mathcal{N}^{\circ}} \operatorname{supp} \lambda_{p}.$$
(2.5)

Remark 2.1 It is well–known (c.f. [19, 20]) that for arbitrarily given initial iterate $u^{(0)}$ the iterates $u^{(\nu)}$, $\nu \geq 1$, converge monotonically decreasingly to the solution u of (2.1) provided that the finite element discretization is monotone. Note that in three dimensions this condition may be violated even if the underlying triangulation satisfies the Delaunay condition that the circumsphere of the four vertices of any tetrahedron in the triangulation contains no vertices in its interior [29]. However, there is numerical evidence that even the approximate solution of the reduced subproblems (2.4) up to some accuracy κ leads to satisfying results if κ is chosen small enough. The actual choice of κ which seems to depend on regularity properties of the problem is still an open question.

In the inexact case, the convergence of a related most constrained strategy has been proved in [18], providing a stopping criterion for the inner iteration. However, this strategy turns out to be much too pessimistic in actual computations leading to a prohibitive large number of outer iteration steps.

Following [23] the reduced linear subproblems will be solved approximately by preconditioned conjugate gradient iteration. For basic information about the preconditioned cg-method we refer to [2] while the construction of appropriate multilevel preconditioners will be considered in the next section.

Chapter 3

Reduced BPX Preconditioning

Let \mathcal{T}_0 be an intentionally coarse conforming triangulation of Ω . Based on some refinement criterion the partition \mathcal{T}_0 is refined several times providing a sequence of triangulations and a corresponding sequence of finite element spaces. The underlying refinement algorithm is a straightforward extension of the well–established red/green refinement technique proposed in [5] to three space dimensions. To provide a regular (red) refinement of some tetrahedron t, first the edges of t are bisected as shown in Figure 3.1 leading to a partition in four similar sub–tetrahedra and an octahedron. To preserve the shape



Figure 3.1: Regular Refinement of the Triangular Faces

regularity of the elements, the remaining octahedron is subdivided according to the strategy of Bey [6] (see Figure 3.2). After local regular refinement we use three different types of irregular (green) closures depicted in the Figures 3.3–3.5 to obtain a conforming triangulation. For a detailed description of the refinement algorithm we refer to [8].

As usual, a refined tetrahedron is said to be the father of its sub-tetrahedra,



Figure 3.2: Splitting of the Remaining Octahedron in Four Tetrahedra w.r.t. the Diagonal (5,9)

which are in turn called sons. The depth of a tetrahedron is given by the number of its ancestors. Finally, the tetrahedra of the initial triangulation \mathcal{T}_0 together with all tetrahedra resulting from regular refinement are called regular, while irregular refinement leads to irregular tetrahedra. Using the hierarchical data structures described for instance in the 3-D ELLKASK



Figure 3.3: Green-I Closure

programmer's manual [17] the triangulations produced by this dynamic refinement process are stored as a sequence $\mathcal{T}_0, \mathcal{T}_1, \dots, \mathcal{T}_j$ with the following properties.

- (T1) Each vertex of \mathcal{T}_{k+1} which does not belong to \mathcal{T}_k , is a vertex of a regular tetrahedron, $0 \leq k < j$.
- (T2) Irregular tetrahedra have no sons.
- (T3) The father of each tetrahedron $t \in \mathcal{T}_{k+1} \setminus \mathcal{T}_k$ has depth k, $0 \le k < j$.

The rule (T3) allows for the reconstruction of the whole sequence $\mathcal{T}_0, \mathcal{T}_1, \dots, \mathcal{T}_j$ with the properties (T1)–(T3) from the initial triangulation \mathcal{T}_0 and the actual triangulation \mathcal{T}_j alone. We emphasize that in general this sequence does not reflect the dynamic refinement process. For further information we refer to [8, 23] and the literature cited therein.

Due to the rules (T1 – T3) the sequence S_0, \ldots, S_j of finite element spaces corresponding to T_0, \ldots, T_j is nested in the sense that

$$\mathcal{S}_0 \subset \mathcal{S}_1 \subset \ldots \subset \mathcal{S}_j. \tag{3.1}$$

Now assume that we have a disjoint splitting $\mathcal{N}_j = \mathcal{N}_j^{\bullet} \cup \mathcal{N}_j^{\circ}$ which may result from an active set strategy applied to (2.1). The remainder of this section will be devoted to the construction of an efficient multilevel preconditioner for the corresponding reduced system

Find
$$u_j^{\circ} \in \mathcal{S}_j^{\circ}$$
 such that $a(u_j^{\circ}, v) = \ell(v) - a(u_j^{\bullet}, v)$, $v \in \mathcal{S}_j^{\circ}$. (3.2)



Figure 3.4: Green-II Closure

Following [38, 7, 23] the analysis will be carried out in the framework of additive Schwarz methods. Apparently, this approach was initiated in [14] and meanwhile became standard in the theory of multilevel methods. For excellent overviews we refer to [34, 37].

To provide an appropriate multilevel splitting of the reduced finite element space S_j° , we first derive a sequence of finite element spaces S_k° , $0 \leq k < j$, which is nested in the sense of (3.1). For $0 < k \leq j$, let $\mathcal{N}_{k-1}^{\circ}$ be the set of all nodes $p \in \mathcal{N}_{k-1} \cap \mathcal{N}_k^{\circ}$ whose k-neighbors $q \in \mathcal{N}_k \setminus \mathcal{N}_{k-1}$ are also contained in \mathcal{N}_k° and let $\mathcal{N}_{k-1}^{\bullet} = \mathcal{N}_{k-1} \setminus \mathcal{N}_{k-1}^{\circ}$. As usual, $p, q \in \mathcal{N}_k$ are called k-neighbors if there is an edge $e = (p, q) \in \mathcal{E}_k$. Now the reduced coarse-grid spaces \mathcal{S}_k° are defined as follows

$$\mathcal{S}_k^{\circ} = \{ v \in \mathcal{S}_k \mid v(p) = 0, \ p \in \mathcal{N}_k^{\bullet} \} , \quad 0 \le k \le j.$$
(3.3)

Note that the definition (3.3) may be replaced by

$$v \in \mathcal{S}_k^{\circ} \Leftrightarrow v \in \mathcal{S}_k \text{ and } \operatorname{supp} v \subset \Omega_j^{\circ},$$

$$(3.4)$$

using the reduced computational domain $\Omega_j^{\circ} = \bigcup_{p \in \mathcal{N}_j^{\circ}} \operatorname{supp} \lambda_p^{(j)}$. From (3.4) it is obvious that

$$\mathcal{S}_0^\circ \subset \mathcal{S}_1^\circ \subset \ldots \subset \mathcal{S}_j^\circ \tag{3.5}$$

so that a multilevel splitting of S_j° can be performed in a straightforward way. In particular we chose the following sets of nodal basis functions,

$$\Lambda_0 = \{\lambda_p^{(0)} | \ \lambda_p^{(0)} \in \mathcal{S}_0^\circ\}$$



Figure 3.5: Green-III Closure

$$\Lambda_H = \bigcup_{k=1}^{j} \Lambda_k , \quad \Lambda_k = \{ \lambda_p^{(k)} | \ \lambda_p^{(k)} \in \mathcal{S}_k^{\circ} \setminus \mathcal{S}_{k-1}^{\circ} \} , \ 1 \le k \le j,$$

and define a multilevel splitting

$$\mathcal{S}_j^\circ = V_0 + \sum_{\lambda \in \Lambda_H} V_\lambda \tag{3.6}$$

into the subspaces

$$V_0 = \operatorname{span}\{\lambda \mid \lambda \in \Lambda_0\}, \quad V_\lambda = \operatorname{span}\{\lambda\}, \ \lambda \in \Lambda_H.$$
(3.7)

Applying the well-known machinery of additive Schwarz methods (see for example [15]) to the multilevel splitting (3.6) we obtain a reformulation

$$Pu_i^\circ = \ell'$$

of the original problem (3.2). Here

$$P = P_0 + \sum_{\lambda \in \Lambda_H} P_\lambda$$

denotes the sum of the Ritz projections $P_{\nu} : \mathcal{S}_{j}^{\circ} \to V_{\nu}, \nu \in \{0, \lambda \in \Lambda_{H}\},$ defined by

$$a(P_{\nu}w,v) = a(w,v) , \ v \in V_{\nu}$$

for each $w \in S_j^{\circ}$ and $\ell' \in (S_j^{\circ})'$ is chosen appropriately. Denoting by (\cdot, \cdot) the standard L^2 -inner product we introduce the L^2 -projections $Q_{\nu} : S_j^{\circ} \to V_{\nu}$

and the representation operators $A_{\nu}: V_{\nu} \to V_{\nu}, \nu \in \{0, \lambda \in \Lambda_H\}$ according to

$$(Q_{\nu}w,v) = (w,v) , v \in V_{\nu}$$

for each $w \in \mathcal{S}_i^\circ$ and

$$(A_{\nu}w, v) = a(w, v) , \quad v \in V_{\nu}$$

for each $w \in V_{\nu}, \nu \in \{0, \lambda \in \Lambda_H\}$. Using the L^2 -representation $A_j : \mathcal{S}_j^{\circ} \to \mathcal{S}_j^{\circ}$ of $a(\cdot, \cdot)$ defined by

$$(A_j w, v) = a(w, v), \quad v \in \mathcal{S}_j^\circ,$$

it is easily verified that $A_{\nu}P_{\nu} = Q_{\nu}A_{j}$. Hence, the operator P may be rewritten as

$$P = H_j A_j$$

where H_j stands for the preconditioner

$$H_j = A_0^{-1} Q_0 + \sum_{\lambda \in \Lambda_H} A_\lambda^{-1} Q_\lambda .$$

Evaluation of $A_{\lambda}^{-1}Q_{\lambda}$ leads to

$$H_j = A_0^{-1} Q_0 + \sum_{\lambda \in \Lambda_H} \frac{(\cdot, \lambda)}{a(\lambda, \lambda)} \lambda .$$
(3.8)

Note that H_j may be regarded as multilevel nodal basis preconditioner (c.f. [34]) based on symmetrically truncated basis functions. A possible unsymmetric truncation has been considered in [23]. Note that in the unconstrained case the preconditioner H_j is reducing to a special formulation of the well-known BPX preconditioner [10]. An efficient implementation of H_j is easily derived along the lines indicated in [8].

If H_j is applied in the context of an active set strategy, the coarse grid space V_0 may change in each outer iteration step. For this reason, it may be useful to replace the evaluation of $A_0^{-1}Q_0$ by simple diagonal scaling. For a further discussion we refer to [34, 37] and the literature cited therein.

The subsequent analysis of the condition number of $P = H_j A_j$ will be guided by the following lemma on additive Schwarz methods.

Lemma 3.1 i) Assume that for all $v \in S_j^{\circ}$ there is a splitting $v = v_0 + \sum_{\lambda \in A_H} v_{\lambda}$ such that

$$c\{a(v_{\theta}, v_{\theta}) + \sum_{\lambda \in \Lambda_H} a(v_{\lambda}, v_{\lambda})\} \le a(v, v)$$
(3.9)

holds for some fixed positive constant c. Then we have the estimate

$$ca(v,v) \le a(Pv,v), v \in \mathcal{S}_j^\circ.$$

ii) Assume that for all splittings $v = v_0 + \sum_{\lambda \in A_H} v_\lambda$ of $v \in S_i^\circ$ the estimate

$$a(v,v) \le C\{a(v_{\theta},v_{\theta}) + \sum_{\lambda \in \Lambda_H} a(v_{\lambda},v_{\lambda})\}$$
(3.10)

holds for some fixed positive constant C. Then we have the estimate

$$a(Pv,v) \le Ca(v,v), \ v \in \mathcal{S}_j^\circ.$$

Proof. The assertion i) is the well-known lemma of P.L. Lions [30]. The simple proof is sketched for completeness. Let $v \in S_j^{\circ}$ and assume that the splitting $v = v_{\theta} + \sum_{\lambda \in \Lambda_H} v_{\lambda}$ satisfies the condition (3.9). Then it follows from the definition of the orthogonal projections P_{ν} , $\nu \in \{0, \lambda \in \Lambda_H\}$, and the Cauchy–Schwarz inequality that

$$a(v,v) \le (a(P_0 v, v) + \sum_{\lambda \in \Lambda_H} a(P_\lambda v, v))^{\frac{1}{2}} (a(v_0, v_0) + \sum_{\lambda \in \Lambda_H} a(v_\lambda, v_\lambda))^{\frac{1}{2}}.$$

Application of (3.9) and the definition of P gives the assertion.

To prove ii) we apply (3.10) to the splitting $Pv = P_0 v + \sum_{\lambda \in A_H} P_\lambda v$ for some fixed $v \in S_j^{\circ}$ to obtain

$$a(Pv, Pv) \le C\{a(P_0v, P_0v) + \sum_{\lambda \in \Lambda_H} a(P_\lambda v, P_\lambda v)\} = Ca(Pv, v)$$

which completes the proof.

The assumptions (3.9) and (3.10) can be regarded as an asymptotic orthogonality of the subspaces V_{ν} , $\nu \in \{0, \lambda \in \Lambda_H\}$. Note that (3.10) is frequently established by strengthened Cauchy–Schwarz inequalities measuring the angles between V_{ν} with respect to $a(\cdot, \cdot)$ or any other symmetric bilinear form which is generating a uniformly equivalent norm on S_i .

In addition to the usual (semi) norms $\|\cdot\|_{\partial}$ and $|\cdot|_{1}$ of $L^{2}(\Omega)$ and $H^{1}(\Omega)$ we will make use of the local (semi) norms $\|\cdot\|_{\partial,\Omega_{0}}$ and $|\cdot|_{1,\Omega_{0}}$ induced by

$$(v, w)_{\Omega_0} = \int_{\Omega_0} v(x) w(x) dx , \quad v, w \in L^2(\Omega_0)$$

and the semi-inner product

$$(v,w)_{1,\Omega_0} = \sum_{i=1}^{3} (\partial_i v, \partial_i w) , \quad v,w \in H^1(\Omega_0)$$

for measurable $\Omega_0 \subset \Omega$. We introduce the L^2 -projection $Q_k : \mathcal{S}_j^{\circ} \to \mathcal{S}_k^{\circ}$ by

$$(Q_k w, v) = (w, v), \quad v \in \mathcal{S}_k^\circ, \quad 0 \le k \le j.$$

and denote the diameter of a tetrahedron t by h(t). For every node $p \in \mathcal{N}_k$ and every tetrahedron $t \in \mathcal{T}_k$ we define $U(p,k) = \operatorname{supp} \lambda_p^{(k)}$ and

$$U(t,k) = \{t' \in \mathcal{T}_k \mid t \cap t' \neq \emptyset\}$$

as the union of all tetrahedra in \mathcal{T}_k intersecting t. Finally, constants depending only on the ellipticity (1.3) and the shape regularity of \mathcal{T}_0 will be denoted by c or C. Other parameters will be indicated explicitly.

We take up the analysis of the preconditioners with the following technical lemma

Lemma 3.2 For some fixed k, $0 < k \leq j$, let $\Lambda_{k-1} = \emptyset$ and $\Lambda_k \neq \emptyset$. Then we have the estimate

$$\sum_{p \in \mathcal{N}_k^{\circ}} |v_k(p)\lambda_p^{(k)}|_1^2 \le C |v_k|_1^2, \quad v_k \in \mathcal{S}_k^{\circ}.$$

Proof. Let $p \in \mathcal{N}_{k-1}$. As $\Lambda_{k-1} = \emptyset$, p is either contained in \mathcal{N}_k^{\bullet} or has at least one k-neighbor $q \in \mathcal{N}_k \setminus \mathcal{N}_{k-1}$ which is contained in \mathcal{N}_k^{\bullet} . Hence, the semi-norm $|\cdot|_1$ is a norm on the restriction of $v_k \in \mathcal{S}_k^{\circ}$ to U(p, k-1). Now it follows from the uniform shape regularity of \mathcal{T}_k and the equivalence of norms on finite dimensional spaces that

$$\sum_{q \in \mathcal{N}_k \cap U(p,k-1)} |v_k(q)\lambda_q^{(k)}|_1^2 \le c |v_k|_{1,U(p,k-1)}^2, \quad v_k \in \mathcal{S}_k^{\circ},$$

Summing up over all $p \in \mathcal{N}_{k-1}$ gives the assertion.

The following assumption is crucial for the stability of the L^2 -projections Q_k .

(Q) There is a constant $c_0 > 0$ independent of j such that for $0 \le k \le j$ and all $t \in \mathcal{T}_k$ with the property $t \cap \mathcal{N}_j^\circ \ne \emptyset$ we have the estimate

$$||v||_{0,U(t,k)} \le c_0 h(t) |v|_{1,U(t,k)}, \quad v \in \mathcal{S}_j^{\circ}.$$
(3.11)

Remark 3.1 Recall that the reduced problem (3.2) may be regarded as a Dirichlet problem on the reduced computational domain Ω_j° . It is the basic source of trouble that in general the boundary of Ω_j° is not represented exactly on lower levels. In particular, we cannot control the shape regularity of U(t, k) intersecting the free boundary so that we cannot derive (3.11) from Poincaré's inequality via local transformations to a finite number of reference configurations as in the neighborhood of $\partial\Omega$ (compare the proof of Lemma 4.1 in [36]). Recall that the boundary $\partial\Omega$ of Ω is known to consist of the faces

of the coarse tetrahedra $t \in \mathcal{T}_{0}$. Hence, the assumption (Q) may regarded as an asymptotic regularity assumption on the discrete free boundary $\partial \Omega_{0}^{\circ} \setminus \partial \Omega$.

Lemma 3.3 Assume that (Q) holds. Then the L^2 -projections Q_k , $0 \le k \le j$, satisfy the error estimate

$$\|v - Q_k v\|_0^2 \le c4^{-k} |v|_1^2, \quad v \in \mathcal{S}_k^{\circ}.$$
(3.12)

Moreover, the Q_k are H^1 -stable in the sense that

$$|Q_k v|_1^2 \le C |v|_1^2, \quad v \in \mathcal{S}_j^{\circ} .$$
(3.13)

The constants c, C depend only on the local geometry of \mathcal{T}_0 and the constant c_0 from (Q).

Proof. The proof follows almost literally the arguments of Yserentant [36] in his proofs of Theorem 4.3 and Theorem 4.5. However, the application of Poincaré's inequality in the proof of Lemma 4.1 has to be replaced by (3.11) if U(t, k) intersects the free boundary.

Now we are ready to state the main result of this section.

Theorem 3.1 Assume that the condition (Q) holds. Then there exist constants K_0 , K_1 depending only on α_0 , α_1 in (1.3), the shape regularity of \mathcal{T}_0 and the constant c_0 in (Q) such that the estimate

$$K_0(j+1)^{-1}a(v,v) \le a(H_jA_jv,v) \le K_1a(v,v)$$

holds for all $v \in \mathcal{S}_i^{\circ}$.

Proof. Let us first consider the lower eigenvalue assuming for the moment that $\Lambda_0 \neq \emptyset$. To verify the assumption of Lemma 3.1 i) we consider the splitting

$$v = Q_0 v_0 + \sum_{k=1}^{j} (Q_k v - Q_{k-1} v)$$
(3.14)

of some fixed $v \in S_j^{\circ}$. It is easily seen that (3.14) gives rise to the representation $v = v_{\theta} + \sum_{\lambda \in A_H} v_{\lambda}$ where $v_{\theta} \in V_{\theta}$ and $v_{\lambda} \in V_{\lambda}$, $\lambda \in \Lambda_H$ are uniquely defined by

$$v_0 = Q_0 v$$
, $Q_k v - Q_{k-1} v = \sum_{\lambda \in \Lambda_k} v_\lambda$, $k = 1, \cdots, j.$ (3.15)

Using the continuity of $a(\cdot, \cdot)$ and the the 3–D counterpart of the inverse inequality in Lemma 3.3 of [36], we have

$$\sum_{\lambda \in \Lambda_H} a(v_{\lambda}, v_{\lambda}) \le \alpha_I \sum_{\lambda \in \Lambda_H} |v_{\lambda}|_I^2 \le c \sum_{k=1}^J 4^k \sum_{\lambda \in \Lambda_k} \|v_{\lambda}\|_0^2.$$
(3.16)

A simple computation gives

$$\sum_{\lambda \in \Lambda_{k}} \|v_{\lambda}\|_{0}^{2} = \frac{1}{10} \sum_{t \in \mathcal{T}_{k} \cap \Omega_{j}^{n}} |t| \sum_{p \in t} |(Q_{k}v - Q_{k-1}v)(p)|^{2} \\ \leq c \|Q_{k}v - Q_{k-1}v\|_{0}^{2}$$
(3.17)

and finally we have from (3.16), (3.17) and Lemma 3.3 that

$$\sum_{\lambda \in \Lambda_H} a(v_{\lambda}, v_{\lambda}) \le c \sum_{k=1}^{j} 4^k \|Q_k v - Q_{k-1} v\|_0^2 \le C(j+1) \|v\|_1^2$$
(3.18)

The proof is completed by the H^1 -stability of Q_0 , i.e.

$$a(v_0, v_0) \le \alpha_1 |Q_0 v|_1^2 \le C |v|_1^2.$$
(3.19)

As by definition $V_0 = \operatorname{span} \Lambda_0$, we still have to consider the case

$$\Lambda_{k^*} \neq \emptyset , \ \Lambda_{k^*-1} = \ldots = \Lambda_0 = \emptyset$$
(3.20)

for some $k^* > 0$. Thus changing the initial level from 0 to k^* we obtain

$$Q_{k^*}v = \sum_{\lambda \in \Lambda_{k^*}} v_{\lambda}$$

so that (3.19) has to be replaced by

$$\sum_{\lambda \in \Lambda_{k^*}} a(v_\lambda, v_\lambda) \le \alpha_I \sum_{p \in \mathcal{N}_{k^*}^{\mathbf{o}}} |v_{\lambda_p^{(k^*)}}|_I^2 \le c |Q_{k^*}v|_I^2$$
(3.21)

which is an immediate consequence of Lemma 3.2 applied to $v_k = Q_k v$. This completes the proof of the lower bound of $a(H_j A_j v, v)$.

To prove an upper bound we can use the same arguments as in [7] and [38] which rely on a suitable coloring of the nodes and a strengthened Cauchy–Schwarz inequality with respect to $(\cdot, \cdot)_{1}$. In particular, we decompose Λ_k according to

$$\Lambda_k = \bigcup_{i=1}^{I} \Lambda_{k,i} \tag{3.22}$$

where the $\Lambda_{k,i}$ are chosen such that

$$\operatorname{supp} \lambda \cap \operatorname{supp} \overline{\lambda} = \emptyset , \ \lambda, \overline{\lambda} \in \Lambda_{k,i}$$

Note that due to the refinement rules (T1) - (T3), this can be achieved by a uniformly bounded number I of subsets $\Lambda_{k,i}$ for each level $k, 0 < k \leq j$. Based on the partition (3.22) we introduce the spaces

$$V_{k,i} = \operatorname{span} \Lambda_{k,i}.$$

Observe that by construction the functions in $V_{k,i}$ are mutually orthogonal. Now chose an arbitrary splitting of some fixed $v \in S_j^{\circ}$ in contributions from the subspaces V_0 and V_{λ} , $\lambda \in \Lambda_H$

$$v = v_0 + \sum_{\lambda \in \Lambda_H} v_\lambda. \tag{3.23}$$

Based on the partition (3.22) the splitting (3.23) can be rewritten in the form

$$v = v_0 + \sum_{k=1}^{j} \sum_{i=1}^{I} v_{k,i} , \quad v_{k,i} = \sum_{\lambda \in \Lambda_{k,i}} v_\lambda \in V_{k,i}$$

so that the assertion is an immediate consequence of

$$|v|_{I}^{2} \leq C\left(|v_{0}|_{I}^{2} + \sum_{k=1}^{j} \sum_{i=1}^{I} |v_{k,i}|_{I}^{2}\right)$$
(3.24)

exploiting the orthogonality of $v_{\lambda} \in \Lambda_{k,i}$. However, (3.24) follows from the strengthened Cauchy–Schwarz inequality

$$(v_k, w_l)_1 \le c \left(\frac{1}{\sqrt{2}}\right)^{l-k} |v_k|_1 |w_l|_1$$
 (3.25)

for $v_k \in S_k^\circ$, $w_l \in V_{l,i}$ and l > k which can be derived by standard arguments used for example in [7, 35]. This completes the proof of the theorem.

The estimate derived in Theorem 3.1 is suboptimal compared to the O(1) – results due to [31], [12] and [9]. The corresponding investigation of minimal regularity assumptions on the free boundary which still allow for optimal condition number estimates will be subject of further research.

However, even in the unconstrained case it frequently happens that the refinement process is stopped for accuracy reasons before the saturation of the condition number occurs. This observation is supported by the numerical results presented in the final section.

Chapter 4

A Posteriori Error Estimates

Let $u \in H_0^1(\Omega)$ denote the exact solution of (1.2), $u_j \in S_j$ the exact solution of the approximate problem (2.1) and $\tilde{u}_j \in S_j$ an approximate solution of (2.1). In particular, \tilde{u}_j may result from a certain number of steps of some iterative solver applied to (2.1). As only \tilde{u}_j is known in actual computations, we are interested in local a posteriori error estimates for the total error $\varepsilon :=$ $\|u - \tilde{u}_j\|$ using the energy norm $\|\cdot\| = a(\cdot, \cdot)^{1/2}$ induced by the actual bilinear form. The local contributions to the total error will be utilized as local error indicators in the adaptive refinement process.

For an overview on the variety of well–established concepts in the unconstrained case we refer to [8, 13, 24, 32, 33] and the literature cited therein. Meanwhile there are some generalizations to variational inequalities of obstacle type. See for example [1, 25, 23, 26, 27].

In the present paper we will follow the basic approach of [13] which has been already successfully applied to obstacle problems (see e.g. [23, 26, 27]) to derive a posteriori estimates $\tilde{\varepsilon}$ which are reliable and efficient in the sense that

$$\gamma_0 \tilde{\varepsilon} \le \|u - \tilde{u}_j\| \le \gamma_I \tilde{\varepsilon} \tag{4.1}$$

holds with positive constants γ_0 , γ_1 independent of j. In particular, we will proceed in two main steps:

- Step 1: Approximate the defect problem by piecewise quadratic finite elements.
- Step 2: Approximate the resulting discrete defect problem by a semilocal or local simplification.

We introduce the subspace $Q_j \subset H^1_0(\Omega)$ of continuous, piecewise quadratic functions vanishing at the boundary and the corresponding approximation

$$K_j^{\mathcal{Q}} = \left\{ v \in \mathcal{Q}_j | v(p) \le \varphi^L(p), p \in \mathcal{N}_j, v(e) \le \varphi^Q(e), e \in \mathcal{E}_j \right\}$$

of the constraints K. Here we used $v(e) := v(\text{midpoint of } e), \ e \in \mathcal{E}_j$, for functions $v : \Omega \to \mathbb{R}$ and suitable restrictions φ^L , φ^Q of the obstacle φ to \mathcal{N}_j and \mathcal{E}_j , respectively. Recall that \mathcal{E}_j is denoting the set of interior edges of \mathcal{T}_j . The piecewise quadratic approximation $U_j \in K_j^Q$ of u is obtained from

Find
$$U_j \in K_j^{\mathcal{Q}}$$
 such that $a(U_j, U_j - v) \le \ell(U_j - v)$, $v \in K_j^{\mathcal{Q}}$. (4.2)

For notational convenience the index j will be suppressed in the following notations. Now the approximate error $d = U_j - \tilde{u}_j \in \mathcal{Q}_j$ may be computed from (4.2) or directly from the following defect problem

Find
$$d \in D$$
 such that $a(d, d-v) \le r(d-v)$, $v \in D$. (4.3)

The constraints are given by

$$D = D(\tilde{u}_j) := \{ v \in \mathcal{Q}_j | v + \tilde{u}_j \in K_j^{\mathcal{Q}} \}$$

and the right-hand side is the residual $r := \ell - a(\tilde{u}_j, \cdot)$.

In Step 2 we concentrate on the simplification of (4.3) replacing $a(\cdot, \cdot)$ by a suitable quadratic form $\tilde{a}(\cdot, \cdot)$. For this reason, we introduce the two-level splitting

$$\mathcal{Q}_j = \mathcal{S}^L \oplus \mathcal{S}^Q \tag{4.4}$$

consisting of the linear part $S^L = S_j$ and the remaining quadratic part $S^Q = \operatorname{span}\{\mu_e | e \in \mathcal{E}_j\}$, where the quadratic bubbles $\mu_e \in \mathcal{Q}_j$ are defined by $\mu_e(p) = 0, p \in \mathcal{N}_j$, and $\mu_e(\bar{e}) = \delta_{e,\bar{e}}, \bar{e} \in \mathcal{E}_j$ (Kronecker delta). This splitting is independent of the space dimension. Utilizing the representation $v = v_L + \sum_{e \in \mathcal{E}_j} v_e \mu_e, v \in \mathcal{Q}_j$, the quadratic form $\tilde{a}(\cdot, \cdot)$ is defined by

$$\tilde{a}(v,w) = a(v^L, w^L) + \sum_{e \in \mathcal{E}_j} v_e w_e a(\mu_e, \mu_e) , \quad v, w \in \mathcal{Q}_j.$$

$$(4.5)$$

It is well-known from [8, 13] that $a(\cdot, \cdot)$ and $\tilde{a}(\cdot, \cdot)$ are spectrally equivalent in the sense that

$$c\tilde{a}(v,v) \le a(v,v) \le C\tilde{a}(v,v), \quad v \in \mathcal{S}_j.$$

$$(4.6)$$

Now we can state the main result of this section.

Theorem 4.1 Assume that the piecewise quadratic approximation $U_j \in Q_j$ is of higher accuracy than the piecewise linear approximation $u_j \in S_j$ in the sense that

$$||u - U_j|| \le q ||u - u_j|| , \ 0 \le q < 1 ,$$
(4.7)

and that $\tilde{u}_j \in \mathcal{S}_j$ satisfies

$$\|u - u_j\| \le \sigma \|u - \tilde{u}_j\| \tag{4.8}$$

with $q\sigma < 1$ and q, σ not depending on j. Let \tilde{d} be the solution of the semi-local problem

Find $\tilde{d} \in D$ such that $\tilde{a}(\tilde{d}, \tilde{d} - v) \le r(\tilde{d} - v)$, $v \in D$. (4.9)

Then (4.1) holds for $\tilde{\varepsilon}$ defined by

$$\tilde{\varepsilon}^2 = \tilde{a}(\tilde{d}, \tilde{d}) \tag{4.10}$$

and constants γ_0 , γ_1 depending only on $q\sigma$, the ellipticity of $a(\cdot, \cdot)$ and the shape regularity of \mathcal{T}_0 .

Proof. Theorem 4.1 is an immediate consequence of the Lemmas 4.1 and 4.2 in [23].

Note that it is a sufficient condition for (4.8) that

$$||u_j - \tilde{u}_j|| \le (1 - 1/\sigma) ||u - u_j||.$$

holds with $\sigma < q^{-1}$. This may be regarded as an accuracy assumption on \tilde{u}_j . For a further discussion of (4.7) and (4.8) we refer to [23].

The error estimate (4.9) is called semi–local, because \tilde{d}^L and \tilde{d}^Q are decoupled with respect to the quadratic form but coupled by the set of constraints.

In our numerical experiments we will use the local contributions

$$\eta_e = (\tilde{d}_e^Q)^2 a(\mu_e, \mu_e) , \quad e \in \mathcal{E}_j$$
(4.11)

of $a^Q(\tilde{d}^Q, \tilde{d}^Q)$ as local error indicators in the adaptive refinement process. As we cannot expect the active region of the continuous defect problem to coincide with the active region of the simplified discretization (4.9) there are no local variants of the inclusion (4.1). Indeed, consider a linear obstacle function φ and let $u = \varphi$ on some tetrahedron t. Then it is not clear that the corresponding indicators η_e vanish though it is known from Theorem 4.1 that asymptotically they cannot be too large. This explains why the semi-local estimate sometimes tends to be too pessimistic.

In practical computations (4.9) may be solved approximately using the active set strategy described above. To provide a good initial iterate the linear and the quadratic part in (4.9) are decoupled by one Gauss – Seidel step applied to the initial iterate zero. More precisely, we compute an estimate $\delta = \delta^L + \delta^Q$ from

Find
$$\delta^L \in D^L$$
 such that $a(\delta^L, \delta^L - v) \le r^L(\delta^L - v)$, $v \in D^L$ (4.12)

and

Find
$$\delta^Q \in D^Q(\delta^L)$$
 such that
 $a^Q(\delta^Q, \delta^Q - v) \le r^Q(\delta^Q - v), \quad v \in D^Q(\delta^L)$
(4.13)

where r^L , r^Q denote the restriction of r to $\mathcal{S}^L, \mathcal{S}^Q$ and $D^L, D^Q(\delta^L)$ are defined by

$$D^L = \mathcal{S}^L \cap D , \quad D^Q(w^L) = \{ v^Q \in \mathcal{S}^Q | v^Q + w^L \in D \} , \quad w^L \in \mathcal{S}^L.$$

Note that in the case of

$$K_j = \{ v \in \mathcal{S}_j | v(p) \le \varphi^L(p), p \in \mathcal{N}_j \} \subset K_j^{\mathcal{Q}}$$

the linear defect problem is recovered by (4.12) with the consequence

$$\delta^L = u_j - \tilde{u}_j$$

Moreover, each component δ_e^Q of δ^Q can be computed separately, giving

$$\delta_e^Q = \min\{r^Q(\mu_e)/a(\mu_e,\mu_e), \ (\varphi^Q - \delta^L - \tilde{u}_j)(e)\}, \ e \in \mathcal{E}_j.$$
(4.14)

Remark 4.1 Assuming that $K_j \subset K_j^{\mathcal{Q}}$ and that the iterative error δ^L is known, we obtain the local error estimate $\tilde{\varepsilon}^2 := \tilde{a}(\delta, \delta)$ introduced in [26]. As a consequence of the theoretical and numerical considerations in [23] this estimate is likely to underestimate the error, but works very satisfactory as soon as the reduced domain $\Omega^\circ = \{\mathbf{x} \in \Omega | u(\mathbf{x}) < \varphi(\mathbf{x})\}$ is resolved properly by the discretization Ω_j° .

Chapter 5

Numerical Results

We consider the elasto-plastic torsion of a cylindrical bar $\Omega = (0, 1)^3$ which is twisted at its upper end around the longitudinal axis in such a way that the lateral surface remains stress free. Modelling the plastic region according to the von Mises yield criterion and normalizing physical constants, it is wellknown (e.g. [16]) that for positive twist angle C per unit length the stress potential u is the solution of the variational inequality (1.2) with $a(\cdot, \cdot), \ell(\cdot)$ given by

$$a(v, w) = (v, w)_{1}, \quad \ell(v) = 2C \int_{\Omega} v \ d(x, y)$$

and the constraints K,

$$K = \{ v \in V | v(\mathbf{x}) \le \operatorname{dist}(\mathbf{x}, \Gamma_{\theta}), \text{ a.e. in } \Omega \},\$$

with $\Gamma_{\theta} = \{\mathbf{x} \in \partial \Omega \mid \mathbf{x} = (x, y, z), 0 < z < 1\}$ denoting the vertical faces of the bar. The solution space V consists of all functions $v \in H^{1}(\Omega)$ satisfying homogeneous Dirichlet conditions at Γ_{θ} . The inactive part $\Omega^{\circ} = \{\mathbf{x} \mid u(\mathbf{x}) < dist(\mathbf{x}, \Gamma_{\theta})\}$ of Ω characterizes the elastic region, while the material is considered plastic in the active points. Note that the elastic region becomes arbitraryly small for increasing C providing a challenging test example both for the preconditioner and the adaptive algorithm.

Of course, there is an equivalent 2–D formulation of this problem which has been already considered in the context of multilevel methods [23]. In the present paper the adaptive multilevel algorithm described in the sequel is applied to the 3–D formulation to allow for a comparison with these former results.

On each refinement level j we apply the active–set strategy described in Section 2 until the active set remains invariant. The iteration is started with the interpolated approximation from the previous level where the value at each node having at least one active neighbor is projected to the obstacle. On the first level the obstacle function is used as initial iterate. Each step of the outer iteration requires the solution of the linear subproblem (2.4) which is performed iteratively by cg-iterations preconditioned by the reduced BPX preconditioner introduced in Section 3. This inner iteration is stopped as soon as the estimated linear iteration error κ satisfies $\kappa \leq \kappa_{\theta}$. Here estimate κ is computed as described in [8]. Recall that the threshold κ_{θ} has to be chosen small enough to ensure the convergence of the outer iteration (c.f. Remark 2.1). In the following computations $\kappa_{\theta} = 10^{-4}$ is used. The same algorithm with $\kappa_0 = 10^{-2}$ is applied to the semi-local defect problem (4.9) providing local error indicators $\eta_e, e \in \mathcal{E}_j$ and an inexact semi-local error estimate $\tilde{\varepsilon}$ according to (4.11) and (4.10), respectively. As initial iterate we use $\delta^Q \in \mathcal{Q}_j$ which is computed from the local obstacle problems (4.14). Recall from Remark 4.1 that δ^Q gives rise to a local error estimate. Now a tetrahedron $t \in \mathcal{T}_j$ is marked for refinement if for at least one edge eof t the contribution η_e exceeds a certain threshold $\sigma \bar{\eta}$. We determine $\bar{\eta}$ by extrapolation as proposed in [3] (see [26] for details) and choose $\sigma = 0.5$.



Figure 5.1: Initial Triangulation \mathcal{T}_0

Level	Depth	Nodes	Iterations	
			Solution	Error Estimate
0	0	27	1/0.0	3/1.7
1	1	125	3/2.3	3/2.0
2	2	223	5/3.3	3/2.7
3	3	665	4/6.3	2/0.0
4	4	2715	4/7.8	2/0.0
5	4	5651	4/8.8	3/0.7
6	5	29773	4/8.3	2/0.0
7	6	44075	5/7.6	2/0.0

 Table 5.1: Iteration History



Figure 5.2: Final Triangulation \mathcal{T}_{γ} on the Cutting Plane z = 0.5



Figure 5.3: Final Solution and Free Boundary on the Cutting Plane z = 0.5

Starting with the initial triangulation \mathcal{T}_0 depicted in Figure 5.1 and choosing C = 5, no elastic region is detected on the initial level. Note that in this case the local error estimates (4.14) provide the start iterate zero which obviously is a too optimistic guess. Compare the corresponding theoretical results and numerical observations in [23].



Figure 5.4: Final Approximation of the Elastic Region



Figure 5.5: Behavior of the Error Estimate

The algorithm is producing the final triangulation \mathcal{T}_{γ} with maximal depth j = 6 and the subscript now indicating the number of 7 refinement steps. The Figures 5.2 and 5.3 show the triangular faces and the level curves of the solution at the cutting plane z = 0.5. Note that the free boundary is emphasized by shading the faces of all tetrahedra which are fully contained



Figure 5.6: Behavior of the Reduced BPX Preconditioner

in the plastic region. Obviously the refinement concentrates on the elastic part where the solution cannot represented by piecewise linear functions. Though the refinement concentrates on the elastic region the semi-local error indicators seem to be too pessimistic introducing points in the plastic part of Ω here and there. Recall the discussion in the previous section.

A picture of the complete free boundary of the elastic region Ω_{γ}° is shown in Figure 5.4.

The behavior of the semi-local and local a posteriori error estimates up to refinement level 5 is illustrated in Figure 5.5 in comparison with the "exact" error resulting from a uniform refinement of \mathcal{T}_5 . As mentioned above the local estimate fails on the initial level but works quite satisfactory later on.

For a detailed history of the solution process we refer to Table 5.1 . The data are presented in the form "number of outer iterations / average number of inner iterations" both needed for the solution and the semi–local error estimate, respectively. Observe that the semi–local error estimate reduces to the local error estimate with increasing refinement. Indeed, the outer iterations do not change the initial guess and may be skipped.

To illustrate the behavior of the reduced BPX preconditioner in more detail, we choose κ_0 unreasonable small, i.e., $\kappa_0 = 10^{-8}$ and the initial iterate is fixed to zero for all inner iterations. In this case the number of (preconditioned) iterations may be used as a measure of the condition number of the corresponding linear system. For each refinement level we choose the linear sub-problem requiring the maximal number of (preconditioned) cg-iteration steps which are reported as a function of the number of unknowns in Figure 5.6 . As expected from the theoretical considerations we observe a linear increase of the number of multilevel preconditioned iterations while without preconditioning the number of iterations grows exponentially with increasing refinement. Obviously, this behavior occurs as soon as the resolution of the elastic region allows for an adequate representation on coarser triangulations. We emphasize that due to Lemma 3.2 the condition number cannot be too bad before this situation is reached.

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