A POSTERIORI ERROR ANALYSIS AND ADAPTIVE FINITE ELEMENT SOLUTION OF VARIATIONAL INEQUALITIES OF THE SECOND KIND

by

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CERTIFICATE OF APPROVAL

PH.D. THESIS

This is to certify that the Ph.D. thesis of

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To my parents, Ion and Dorina

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ABSTRACT

In the employment of the finite element method (and other numerical methods) for solving application problems, an important issue is to assess the reliability of the numerical solution. A posteriori error estimates provide quantitative information on the accuracy of the numerical solution and are the basis for the development of automatic, adaptive procedures for engineering applications of the finite element method.

We perform an a posteriori error analysis for adaptive finite element solution of elliptic variational inequalities of the second kind. Using duality theory in convex analysis, we establish a general framework for a posteriori error estimation. We then derive a posteriori error estimates of residual type and of gradient recovery type, with particular choices of the dual variable present in the general framework. The reliability of the error estimates is rigorously shown. The efficiency of the error estimators is theoretically investigated and numerically validated. Detailed derivation and analysis of the error estimates are given for a model variational inequality of the second kind.

We present extension of the results in solving other elliptic variational inequalities such as those arising in the study of frictional contact problems in elasticity. First, we derive a posteriori error estimates for a static frictional contact problem, and then consider a quasistatic case.

We report numerous numerical examples, illustrating the effectiveness of the a posteriori error estimates.

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An Abstract

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CHAPTER 1
PRELIMINARIES

1.1 Introduction

The finite element method today is the dominant numerical method for solving most problems in structural and fluid mechanics. It is widely applied to both linear and nonlinear problems. General mathematical theory of finite element methods can be found in [4, 28, 29, 59, 66], among others. The textbook [52] offers an easily accessible mathematical introduction of finite element methods, whereas the two recent textbooks, [19, 20], provide deeper mathematical theory together with more recent and current research development such as the multigrid methods. Traditionally, convergence of finite element solutions is achieved through mesh refinement with the use of piecewise low degree polynomial. Since h is usually used to denote the mesh size, the traditional finite element method is also termed as the h-version finite element method. Convergence of the method can also be achieved by using piecewise increasingly higher degree polynomials over relatively coarse finite element meshes, leading to the p-version finite element method. Detailed discussion of the p-version finite element method can be found in [68]. The p-version method is more efficient in areas where the solution is smooth, so it is natural to combine the ideas of the p-version and the h-version to make the finite element method very efficient on many problems. A well-known result regarding the h-p-version finite element method is the exponential convergence rate for solving elliptic boundary value problems with corner singularities. Comprehensive mathematical theory of the p-version and h-p-version finite element methods with applications in solid and fluid mechanics can be found in [65]. Mixed and hybrid finite element methods are often used in solving boundary value problems with constraints and higher order differential equations. Mathematical theory of these methods can be found in [21, 64]. Several monographs are available on the numerical solution of Navier-Stokes equations by the finite element method, see e.g. [35]. Theory of the finite element method for solving parabolic problems can be found in [69] and more recently in [70]. Finally, we list a few representative engineering books on the finite element method, [11, 51, 79, 80]. The reader is referred to two historical notes [58, 78] on the development of the finite element method.

For practical use of a numerical method, one important issue is the assessment of the reliability and accuracy of the numerical solution. The reliability of the numerical solution hinges on our ability to estimate errors after the solution is computed; such an error analysis is called a posteriori error analysis. A posteriori error estimates provide quantitative information on the accuracy of the solution and are the basis for the development of automatic, adaptive solution procedures.

The research on a posteriori error estimation and adaptive mesh refinement for the finite element method began in the late 1970's. The pioneering work on the topic was done in [5, 6]. Since then, a posteriori error analysis and adaptive computation in the finite element method have attracted many researchers, and a variety of different a posteriori error estimates have been proposed and analyzed. In a typical a posteriori error analysis, after a finite element solution is computed, the solution is used to compute element error indicators and an error estimator. The element error indicator represents the contribution of the element to the error in the computation of some quantity by the finite element solution, and is used to indicate if the element needs to be refined in the next adaptive step. The error estimator provides an estimate of the error in the computation of the quantity of the finite element solution, and thus can be used as a stopping criterion for the adaptive procedure. Often, the error estimator is computed as an aggregation of the element error indicators, and one usually only speaks of error estimators. Most error estimators can be classified into residual type, where various residual quantities (residual of the equation, residual from derivative discontinuity, residual of material constitutive laws, etc.) are used; and recovery type, where a recovery operator is applied to the (discontinuous) gradient of the finite element solution and the difference of the two is used to assess the error. Error estimators have also been derived based on the use of hierarchic bases or equilibrated residual. Two desirable properties of an a posteriori error estimator are reliability and efficiency. Reliability requires the actual error to be bounded by a constant multiple of the error estimator, up to perhaps a higher order term, so that the error estimator provides a reliable error bound. Efficiency requires the error estimator to be bounded by a constant multiple of the actual error, again perhaps up to a higher order term, so that the actual error is not over-estimated by the error estimator. The study and applications of a posteriori error analysis is a current active research area, and the related publications grow fast. Some comprehensive summary accounts can be found, in chronological order, in [73], [1], and [7].

Initially, a posteriori error estimates were mainly developed for estimating the finite element error in the energy norm. In the recent years, error estimators have also been developed for goal-oriented adaptivity. The goal-oriented error estimators are derived to specifically estimate errors in quantities of interest, other than the energy norm errors. Chapter 8 of [1] is devoted to such error estimators. The latest development in this direction is depicted in [10, 34].

Most of the work so far on a posteriori error analysis has been devoted to ordinary boundary value problems of partial differential equations. In applications, an important family of nonlinear boundary value and initial-boundary value problems is that associated with variational inequalities, that is, problems involving either differential inequalities or inequalities over boundaries or sub-domains. Mechanics is a rich source of variational inequalities (cf. e.g. [60]), and some examples of problems that give rise to variational inequalities are obstacle and contact problems, plasticity and visco-plasticity problems, Stefan problems, unilateral problems of plates and shells, and non-Newtonian flows involving Bingham fluids. An early comprehensive reference on the topic is [31], where many nonlinear boundary value problems in mechanics and physics are formulated and studied in the framework of variational inequalities. A concise introduction to the mathematical theory of some variational inequalities can be found in [55]. Numerical approximations of general variational inequalities are studied in detail in [36, 37]. Numerical methods for some variational inequalities arising in mechanics are the subject of [48, 49]. Mathematical analysis and numerical approximations of variational inequalities arising in contact mechanics are presented in [54] (for elastic materials) and [47] (for viscoelastic and viscoplastic materials). In [44, 45], elastoplasticity problems are formulated and analyzed in the form of variational inequalities.

Although several standard techniques have been developed to derive and analyze a posteriori error estimates for finite element solutions to problems in the form of variational equations, they do not work directly for a posteriori error analysis of numerical solutions to variational inequalities. Nevertheless, numerous papers can be found on a posteriori error estimation of finite element solutions of obstacle problems, e.g., [2], [27], [50], [56], [57], [71] (these papers consider numerical solutions on convex subsets of finite element spaces), as well as [33], [53] (these papers use a penalty approach for discrete solutions). Obstacle problems are so-called variational inequalities of the first kind, that is, they are inequalities involving smooth functionals and are posed over convex subsets. We also note that a posteriori error estimation is discussed in [13, 14, 67], though the arguments in these papers are arguable.

In the context of elastoplasticity with hardening, computable a posteriori error estimates are derived in [3, 22, 24] for the primal problem, which is a variational inequality of the second kind; that is, the inequality arises as a result of the presence of a non-differentiable functional. These works deal extensively also with a priori estimates, and in the latter work a number of numerical examples are presented. Residual type error estimators were studied for an elliptic variational inequality of the second kind in [17, 18].

In this thesis, we derive and study some a posteriori error estimates for finite element solutions of elliptic variational inequalities of the second kind. The basic mathematical tool we will use is the duality theory in convex analysis (cf. [32], [76]). Duality theory has been applied to derive efficient a posteriori error estimates for mathematical idealizations of physical and engineering problems (see, e.g., [39], [40]), as well as for some numerical procedures for solving nonlinear problems, such as the regularization techniques in [38], [43] and [46], and the Kačanov iteration method in [41, 42]. In [62, 61], duality theory techniques were used to derive a posteriori error estimates of the finite element method in solving boundary value problems of some nonlinear equations. In these papers, the error bounds are shown to converge to zero in the limit as the meshsize approaches zero; however, no efficiency analysis of the estimates is given.

1.2 Thesis Organization

The remaining part of this thesis is organized as follows:

In Chapter 2 we introduce some basic notations and results concerning function spaces, variational inequalities and duality theory in convex analysis. A model variational inequality of the second kind is introduced together with its finite element discretization and dual formulation.

In Chapter 3 a general framework for a posteriori error estimation is established by using duality theory. We then derive a posteriori error estimates of residual type and of gradient recovery type, with particular choices of the dual variables present in the general framework. The error estimates are shown to be reliable. Efficiency of the error estimates is theoretically investigated and numerically validated.

In Chapter 4 we present an application of our results to frictional contact problems. We consider both static and quasistatic contact processes. Several numerical examples are reported.

CHAPTER 2
MODEL PROBLEM AND DUAL FORMULATION

2.1 Basic Results and Notations

In this section, we introduce some basic results and notations, which will be needed in the subsequent parts of this thesis. We start with a review of function spaces, then we recall some main results regarding convex analysis, variational inequalities and duality theory.

2.1.1 Function spaces

Let Ω be a bounded open domain in $\mathbb{R}^d$, $d \geq 1$, with Lipschitz boundary $\Gamma = \partial\Omega$. The assumption that Ω has a Lipschitz boundary makes it possible to define the outer unit normal vector ν at almost all points of the boundary. A d-tuple $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_d)$ of non-negative integers α_i, $i = 1, \ldots, d$, is called a multi-index and its length is defined as $|\alpha| = \sum_{i=1}^{d} \alpha_i$. If $v : \Omega \to \mathbb{R}$ is a sufficiently smooth function, then $D^\alpha v$ denotes the αth derivative of the function v,

$$D^\alpha v = \frac{\partial^{|\alpha|} v}{\partial x_1^{\alpha_1} \ldots \partial x_d^{\alpha_d}}.$$

Let m be a non-negative integer and $p \in [1, \infty)$. We start with some standard function spaces:

- $C_0^\infty(\Omega)$ denotes the space of all infinitely differentiable real functions with compact support.
- $C^m(\overline{\Omega})$ denotes the set of all real functions defined in Ω, the derivatives of which

up to the order m can be continuously extended on $\overline{\Omega}$. The expression

$$\|v\|_{C^m(\overline{\Omega})} = \sum_{|\alpha| \leq m} \max_{x \in \overline{\Omega}} |D^\alpha v(x)|$$

defines the norm with respect to which $C^m(\overline{\Omega})$ is a Banach space. Further $C^\infty(\overline{\Omega}) = \bigcap_{m=0}^{\infty} C^m(\overline{\Omega})$. Obviously, $C_0^\infty(\Omega) \subset C^\infty(\overline{\Omega})$.

- $L^p(\Omega)$ for $p \in [1, \infty)$ denotes the space of all (equivalence classes of) real measurable functions v in Ω for which $\|v\|_{L^p(\Omega)} \leq \infty$, where

$$\|v\|_{L^p(\Omega)} = \left(\int_\Omega |v|^p \, dx \right)^{1/p}.$$

  In particular, $L^2(\Omega)$ is a Hilbert space equipped with the inner product

$$(v, w)_{L^2(\Omega)} = \int_\Omega vw \, dx.$$

- $L^\infty(\Omega)$ stands for the space of all real essentially bounded measurable functions in Ω. More precisely: $v \in L^\infty(\Omega)$ iff v is measurable and

$$\|v\|_{L^\infty(\Omega)} = \operatorname{ess\,sup}_{x \in \Omega} |v(x)| \leq \infty.$$

- $L^p_{loc}(\Omega)$ denotes the space of all locally p-integrable functions. A function v is a locally p-integrable function if $v \in L^p(\Omega')$ for any proper subset $\Omega' \subset\subset \Omega$. When $v \in L^1_{loc}(\Omega)$, we say v is locally integrable.

To introduce the Sobolev spaces, we first recall the following definition of the weak derivative:

Definition 2.1.1. *Let $v, w \in L^1_{loc}(\Omega)$ and α a multi-index. Then w is called an αth weak derivative of v if*

$$\int_\Omega v(x) D^\alpha \phi(x)\, dx = (-1)^{|\alpha|} \int_\Omega w(x)\phi(x)\, dx \quad \forall \phi \in C_0^\infty(\Omega).$$

A weak derivative, if it exists, is uniquely defined a.e. With the notion of weak derivative, we can introduce Sobolev spaces.

Definition 2.1.2. *Let m be a non-negative integer and $p \in [1, \infty]$. The Sobolev space $W^{m,p}(\Omega)$ is the set of all the functions $v \in L^1_{loc}(\Omega)$ such that for each multi-index α with $|\alpha| \leq m$, the αth weak derivative $D^\alpha v$ exists and $D^\alpha v \in L^p(\Omega)$. The norm in the space $W^{m,p}(\Omega)$ is defined as*

$$\|v\|_{W^{m,p}(\Omega)} = \begin{cases} \left(\sum_{|\alpha| \leq m} \|D^\alpha v\|^p_{L^p(\Omega)}\right)^{1/p}, & p \in [1, \infty), \\ \max_{|\alpha| \leq m} \|D^\alpha v\|_{L^\infty(\Omega)}, & p = \infty. \end{cases}$$

When $p = 2$, we write $H^m(\Omega) \equiv W^{m,p}(\Omega)$.

In order to simplify notations, we replace $\|v\|_{W^{m,p}(\Omega)}$ by $\|v\|_{m,p;\Omega}$. When $p = 2$, we use $\|v\|_{m;\Omega}$ for $\|v\|_{H^m(\Omega)}$. The semi-norm over the space $W^{m,p}(\Omega)$ is

$$|v|_{W^{m,p}(\Omega)} = \begin{cases} \left(\sum_{|\alpha| = m} \|D^\alpha v\|^p_{L^p(\Omega)}\right)^{1/p}, & p \in [1, \infty), \\ \max_{|\alpha| = m} \|D^\alpha v\|_{L^\infty(\Omega)}, & p = \infty. \end{cases}$$

It is known that $W^{m,p}(\Omega)$ is a Banach space and consequently, $H^m(\Omega)$ is a Hilbert space with a canonical inner product

$$(v, w)_{H^m(\Omega)} = \int_\Omega \sum_{|\alpha| \leq m} D^\alpha v(x) D^\alpha w(x)\, dx, \quad v, w \in H^m(\Omega).$$