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Stable numerical methodology for variational inequalities with application in quantitative finance

and computational mechanics

By

Davood Damircheli

Approved by:

Shanti Bhushan (Major Professor) Mohsen Razzaghi Adrian Sescu Eric M.Collins Adrian Sescu (Graduate Coordinator) Jason M.Keith (Dean, Bagley College of Engineering)

A Documentation File Submitted to the Faculty of Mississippi State University in Partial Fulfillment of the Requirements for the Degree of Doctor of Philosophy in Computational Engineering in the Department of Computational Engineering

Mississippi State, Mississippi

December 2022

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2022

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Candidate for Degree of Doctor of Philosophy

Coercivity is a characteristic property of the bilinear term in a weak form of a partial differential equation in both infinite space and the corresponding finite space utilized by a numerical scheme. This concept implies *stability* and *well-posedness* of the weak form in both the exact solution and the numerical solution. In fact, the loss of this property especially in finite dimension cases leads to instability of the numerical scheme. This phenomenon occurs in three major families of problems consisting of advection-diffusion equation with dominant advection term, elastic analysis of very thin beams, and associated plasticity and non-associated plasticity problems. There are two main paths to overcome the loss of coercivity, first manipulating and stabilizing a weak form to ensure that the discrete weak form is coercive, second using an automatically stable method to estimate the solution space such as the Discontinuous Petrov Galerkin (DPG) method in which the optimal test space is attained during the design of the method in such a way that the scheme keeps the coercivity inherently. In this dissertation, A stable numerical method for the aforementioned problems is proposed. A stabilized finite element method for the problem of migration risk problem which

belongs to the family of the advection-diffusion problems is designed and thoroughly analyzed. Moreover, DPG method is exploited for a wide range of valuing option problems under the black-Scholes model including vanilla options, American options, Asian options, double knock barrier options where they all belong to family of advection-diffusion problem, and elastic analysis of Timoshenko beam theory. Besides, The problem of American option pricing, migration risk, and plasticity problems can be categorized as a free boundary value problem which has their extra complexity, and optimization theory and variational inequality are the main tools to study these families of the problems. Thus, an overview of the classic definition of variational inequalities and different tools and methods to study analytically and numerically this family of problems is provided and a novel adjoint sensitivity analysis of variational inequalities is proposed.

Key words: Variational Inequality, Discontinuous Petrov Galerkin, Credit Migration Risk Problem, Quantitative Finance, Solid Mechanics

DEDICATION

To my wife

Lamiae

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I would like to thank my deceased supervisor, Dr. Manav Bhatia, with whom I started this journey and I had to finish it alone. Many thanks are extended to Dr. Shantia and my committee members Dr. Sescu and Dr. Collins for their guidance and support.

I would like to express my profound gratitude to my parents who made so many sacrifices to give me a brighter future. I would also like to thank my sisters Asieh and Roya for always being there for me even though "there" was miles away. Finally, yet importantly, I want to thank my wife who supports me in ways I never knew I needed.

Starkville, MS, USA, Davood

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CHAPTER I

INTRODUCTION

1.1 Introduction

It is well-known in the literature [25] that when some model parameters take extreme values, coercivity loss occurs. In this case, the discrete form of the problem will suffer from instability despite having a well-posed exact solution. In this investigation, we address three families of the problem that they suffer from coercivity loss

- · Advection diffusion with dominant advection term
- · Elastic bending analysis of thin Timoshenko beam
- · Associated plasticity and non-associated plasticity problem

Let's concentrate on the mathematical background pertaining to this problem and loss of coercivity. Besides, we can identify the model parameters that can take extreme values. To start, let's consider the following problem:

find
$$u \in V$$
 such that
 $a_{\beta}(u, v) = f(v), \forall v \in V,$
(1.1)

where *V* is the appropriate Hilbert space, $f \in V'$, and bilinear form $a_{\beta}(, \cdot)$ is a continuous and coercive form on $V \times V$. The bilinear form a_{β} depend on a parameter β that can take arbitrary small values. We assume $||a_{\beta}|| := ||a_{\beta}||_{V}$, and the coercivity constant c_{β} , i.e.,

$$c_{\beta} = \inf_{u \in V} \frac{a_{\beta}(u, u)}{\|u\|_{V}^{2}}.$$
(1.2)

Coercivity loss happens we in (1.1) if

$$\lim_{\beta \to 0} \frac{\|a_{\beta}\|}{c_{\beta}} = \infty, \tag{1.3}$$

so it is well-known that the error estimate for the problem (1.1) on the dense supspace $V_h \subset V$ is as following

$$\|u - u_h\|_V \le \frac{\|a_\beta\|}{c_\beta} c_i h_h \|u\|_{V_h}.$$
(1.4)

Thus when the problem suffers from coercivity loss (1.3), the error estimate will not perform any dominant term of the error. However, the only way to get a finite value for the error estimate (1.4) is to let $h \rightarrow 0$, which is not practical due to the limitation on mesh refinement on the computers. In this investigation, we study these problems and propose a stabilized numerical method for solving these problems. However, before digging into the numerical scheme for solving these problems, let's intuitively see what will happen in the case of loss of coercivity.

1.1.1 Advection-Diffusion Equation with Dominant Advection

In this part we study the advection-diffusion equation for a domain $\Omega \subset \mathbb{R}^2$,

$$-\nu\Delta u + r \cdot \nabla u = f, \quad \forall u \in \Omega, \tag{1.5}$$

with the diffusion coefficient v > 0, the advection velocity $r : \Omega \to \mathbb{R}^2$, and the source term $f : \Omega \to \mathbb{R}$. Considering the bilinear form

$$\begin{cases} \text{find} \quad u \in V \quad \text{such that} \\ a_{\beta}(u, v) = \int_{\Omega} v \Delta u \cdot \Delta v + \int_{\Omega} v(r \cdot \Delta u). \end{cases}$$
(1.6)

we can use $\beta = \frac{\nu}{\|r\|_{L^{\infty}}}$ to measure the relative importance of advection effects. When this parameter is very smaller than one, e.g. $\beta \ll 1$ implies

$$\frac{\|a_{\beta}\|}{c_{\beta}} = O(\frac{\|r\|_{L^{\infty}}}{\nu}) = O(\frac{1}{\beta})$$
(1.7)

which can eventuate in coercivity loss. Figure (1.1) depicts the approximate the solution of (1.6) using finite element method with the advection velocity of r = (1, 0), with homogeneous Dirichlet boundary condition with the different values of diffusion coefficient $v = 10^{-2}$, 10^{-5} , 10^{-10} , 10^{-15} . As we observe in Fig. (1.1) the approximate solution in the four cases presented oscillation is larger as the diffusion coefficient v goes to zero. Indeed, the PDE (1.5) and the governing equation turns into a first-order PDE as the diffusion term is taking small values close to zero. Hence, the loss of coercivity in the case of advection dominant problem shows instability in the form of oscillation in Fig. (1.1).

1.1.2 Very thin Beams

In this section, we briefly study the static Timoshenko equation where the Euler-Bernoulli theory is a special case of this Timoshenko beam theory. According to the beam theory, the governing equations modeling a steady-state Timoshenko beam on a domain $\Omega = [0, L]$ with length L under a transverse load q are as follows

$$\begin{cases} \frac{\partial}{\partial x} \left(E I_A \frac{\partial \theta_y}{\partial x} \right) + G A \kappa \left(\frac{\partial u}{\partial x} - \theta_y \right) = 0, \\ -\frac{\partial}{\partial x} \left(G A \kappa \left(\frac{\partial u}{\partial x} - \theta_y \right) \right) = q, \end{cases}$$
(1.8)

in which u(x, t) is the transverse displacement and θ_y is the rotation angle of the normal to the main surface of the beam. The elastic modulus and shear modulus are shown by *E* and *G* respectively, κ



Figure 1.1: Finite element approximation of an advection-diffusion equation with dominant advection

is the shear correction factor, ρ is the density, and the cross-section area is A, and I_A is the moment of inertia. Dirichlet boundary conditions for the system (5.2) are

$$\begin{cases} D|_{\Gamma_D} = u_D, \\ \theta_y|_{\Gamma_D} = \theta_{y_0}, \end{cases}$$
(1.9)

using *v* as a test function for the normal displacement *u*, and using *w* as a test function for rotational angle, one can find the following weak form for the system (5.2)

$$\begin{cases} \text{Find} \quad (u,\theta) \in V \times V \quad \text{such that} \quad \forall (v,w) \in V \times V, \\ a((u,\theta),(v,w)) = \frac{\eta}{EI} \int_{\Omega} qv. \end{cases}$$
(1.10)

where the bilinear form defines as

$$a((u,\theta),(v,w)) = \int_{\Omega} \eta \theta' w' + \int_{\Omega} (u'-\theta)(v'-w), \qquad (1.11)$$

where $\eta = \frac{2(1+\nu)I}{S_{\kappa}}$, $V = \{v \in H^{1}(\Omega); v(0) = 0\}$, and the product space $V \times V$ has the norm $\|(u,\theta)\|_{V \times V} = \|u\|_{1,\Omega} + \|\theta\|_{1,\Omega}$. One can find more details about existence and uniqueness of the solution of (1.10) and property of the solution in [25] and the references therein. If we consider the parameter β defined in (1.3) simply equal to η in the weak form defined above, we can see that for $\beta \ll 1$, the following statement holds

$$\frac{\|a_{\beta}\|}{c_{\beta}} = O(\frac{1}{\eta}) = O(\frac{1}{\beta}) \gg 1$$

$$(1.12)$$

which leads to coercivity loss. In fact, when the $\eta \ll 1$ it means the ratio between the inertia moment and the section of the beam is small, that is, we are dealing with very thin beams. Fig. (1.2) illustrates the analytical solution and finite element approximation of the problem (5.2) for $\eta = 10^{-2}$, 10^{-3} for displacement *u* and rotation angle θ . As it is observed the instability in the form of losing the accuracy of the approximation happens as the value of η decreases.



Figure 1.2: Comparison between the analytical and finite element solutions, Bending of a Timoshenko beam supported at both sides, with two different thickness h

1.2 Variational Inequalities

Variational inequality is a broad class of problems and is studied in continuum mechanics in the form of plasticity and contact mechanics. Return mapping algorithm is a general and probably the most popular algorithm for solving plasticity problems[79]. The problem of perfect plastic material was first considered by Duvant and Lion[24]. They studied the partial differential equation of elastoplasticity problem. Johnson [47] developed the theorems for existence of plasticity problems, and used variational inequalities to compute solution. The numerical approximation of variational inequality and their corresponding related problems has dramatically increased in the recent years. Weimin and Reddy[34] studied two alternative variational formulation as the primal and dual problems. They defined the primal problem based on a dissipation function, which is a widely used kinematic (displacement-based) formulation. Whereas, the formulation based on yield function is used to define the corresponding dual problem. Gao[31] showed that dual version is an easier approach in non-smooth equilibrium problems. Linear Complementarity problem was used by Stamacchia and Guido[88] in order to solve the quadratic programming problem obtained from Galerkin approximation. Gerhard[81] borrowed the primal-dual interior point method from convex programming to solve the small-deformation, rate-independent elastoplastic response using finite element methods. Krabbenhoft[50] developed a new method based on the second-order cone and semi-definite programming for solution of cam clay plasticity. This new scheme was far more accurate in comparison with the conventional methods where the material point is used to integrate the constitutive equations and a Newton-Raphson like scheme is used to minimize the out-of-balance forces on the structure. However, the Newton-Raphson solver used in this scheme required more iterations than the conventional method. Discrete variational inequality was studied by Weiners

and Wohlmuth[72]. Indeed, they showed that using the classical return mapping algorithm for inequality is equivalent to a semi-smooth Newton method for the nonlinear system of equations. Adaptive methodology based on the finite element method[72, 82, 29, 32] is developed in the hope of analyzing and approximating the solution of elastoplastic problems. Rannacher and Suttmeier[72] benefit from controlling the error obtained from the adjoint solution as a feedback filtering to yield optimal meshes in linear elasticity. Suttmeier[82] proposed a unified framework for refining meshes based on the concept of a-posteriori error estimation and adaptive mesh design for finite element models of variational inequalities in contact problems. Bangerth and his colleagues[29] applied a set of methods for solving large-scale elastoplastic contact problems with hardening. They used active set method for the contact problems, adaptive finite element discretization with linear and quadratic elements as well as a Newton linearization of the plasticity problem to develop an efficient method. In 2016 Ghorashi and Rabczuk[32] developed a goal-oriented error estimation methodology to estimate the solution of three dimensional elastoplastic problem.

There are some classical examples of variational inequalities such as Strang's problems, contact or obstacle problems[83]. Strang's problem is a problem from elasto-plasticity theory in which the imposed constraints are nonlinear. A fundamental model of contact problem in elasticity is Signorini's problem. Mathematical programming has been used as an effective tool in the development of variational inequalities. It has been used by researchers in the field to not only study the existence, uniqueness and properties of the solution, but also to efficiently approximate solution of variational inequalities.

Sensitivity analysis of variational inequality and nonlinear complementarity problem has been broadly investigated for special forms and under specific theoretical assumptions, but one could barely find a unified sensitivity analysis which satisfies both computational and analytical demands. Former studies of sensitivity analysis was performed as a result of Robinson's [75, 76] finding on generalized equations. Sensitivity of variational inequality has been studied by researchers such as Dafermos [15], Harker [36, 37], Kyparisis [52, 54], and Pang [54] and the references therein. Likwise, sensitivity of nonlinear complementarity problem has been developed by authors like Doung [33], Kojima [48], Miller [65], McLinden [62], Megiddo [64], Pang [54], and Robinson [75], [76]. In addition, sensitivity analysis has been studied for special forms of variational inequality. Kyparisis[53] studied finite dimensional variational inequality and nonlinear complementarity problem thanks to Robinson's results. Investigation on perturbed quasi variational inequality was conducted by Noor[69]. Although, there are authors, such as Dafermos[15], who track the sensitivity analysis of variational inequality from a path which was totally different from Robinson's finding. Indeed, Dafermos tried to solve the problem based on direct geometric arguments. It is worth noticing that the aforementioned papers include the existence and uniqueness of perturbed problem of either variational inequality or nonlinear complementarity problem and they suffer form lack of clear computational algorithms and strategies.

Topological sensitivity of problems pertaining to variational inequality has been investigated over the last decade. Hintermüller[38, 42] studied the abstract shape and topology optimization of elliptic and semi-linear variational inequality. However, among variant problems that lead us to a variational inequality, using inelastic material models brings path-dependency into the model which turns computing of design sensitivity to a nontrivial task. Indeed, this complexity is raised due to the fact that material state depend on the whole history of deformation. Alberdi [?] and his colleges developed a unified framework for adjoint sensitivity of problem involving inelastic materials based on the return mapping algorithm.

In this section, first we present a brief review of variational inequalities and interconnected problems like quadratic programming problem, complementarity problems, fixed-point problem and Wiener-Hopf equation. Approximating the variational inequality using a finite element space, we present the finite dimensional variational inequalities and related problems. Besides, a prototype plasticity problem with linear hardening as an application of variational inequalities is investigated through semi-smooth analysis. Indeed, using the projection approach, the mixed variational inequality of plasticity problem reduces to a primal problem, and formal linearization paves our way to use iterative method such as generalized Newton's method to find the solution of primal problem including non-differentiable projection. In addition, adjoint and direct path-dependence sensitivity of plasticity problem is developed thanks to the same linearization.

1.3 The DPG Method

In this section, we briefly provide a high-level introduction to the Discontinuous Petrov-Galerkin Method with Optimal Test Function. A review of the method is given for the steady-state problem, the transient version of the method with more concrete spaces to treat the specific problems will be presented in the future chapters. Let's begin with the standard well-posed abstract variational formulation which has not necessarily symmetric functional setting, seeking $u \in U$ such that

$$b(u, v) = l(v), \quad v \in V,$$
 (1.13)

where trial space U and test space V are proper Hilbert spaces. $l(\cdot)$ is a continuous linear functional, $b(\cdot, \cdot)$ is a bilinear (sesquilinear) form that satisfies the inf-sup condition as follows:

$$\sup_{v \in V} \frac{|b(u,v)|}{\|v\|_V} \ge \gamma \|u\|_U, \quad \forall u \in U,$$

$$(1.14)$$

which guarantees the well-posedness of the variational form (1.13). However, discretize version of variational form (1.13) with Petrov-Galerkin method is problem of finding $u_h \in U_h \subset U$ such that

$$b(u_h, v_h) = l(v_h), \quad v_h \in V_h, \tag{1.15}$$

Based on Babuška's theorem ([7]) for a discretized system (1.15) in a case where dim (U_h) = dim (V_h) , is stable or to another word the system is well-posed if the discrete inf-sup condition is satisfied as follows

$$\sup_{v_h \in V_h} \frac{|b(u_h, v_h)|}{\|v_h\|_V} \ge \gamma_h \|u_h\|_U, \quad \forall u_h \in U,$$

$$(1.16)$$

where the inf-sup constant γ_h must be bounded away from zero meaning $\gamma_h \ge \gamma > 0$. Now, choosing the discrete spaces of trail and test space is of mater of importance. Indeed, trial space U_h is usually picked by approximability, but trial space V_h can be chosen in such a way to dictate special properties of numerical algorithm such as being well-posed. The Petrov-Galerkin method with optimal test space has been designed in a way that for each discrete function u_h from trial space U_h , it finds a corresponding optimal test function $v_h \in V$ as a supremizer of inf-sup condition, i.e optimal test function $v_h \in V$ construct such that

$$\sup_{v \in V} \frac{|b(u, v)|}{\|v\|_{V}} = \frac{|b(u, v_{h})|}{\|v_{h}\|_{V}}.$$
(1.17)

Given any trial space U_h , let's define a trial-to-test operator $T : U \longrightarrow V$. The optimal test space is defined as the image of the trail space via this operator $V_h^{\text{opt}} := T(U_h)$, where the function from optimal test space $v^{\text{opt}} \in V_h^{\text{opt}}$ is satisfying in

$$(v^{\text{opt}}, v)_V = (Tu_i, v)_V = b(u_i, v), \quad \forall v \in V,$$
 (1.18)

in which $(\cdot, \cdot)_V$ is the inner product on the test space. In fact, the equation (1.18) uniquely determines the optimal test space with Riesz representation theorem with which discrete stability of the discrete form (1.15) automatically is attained. The test function defined in (1.18) is designed in a way that the supremizer of the inf-sup continuous condition implies the satisfaction of the discrete inf-sup condition and as a result, it guarantees the discrete stability. Moreover, we will have

$$\sup_{v_h \in V_h^{\text{opt}}} \frac{|b(u_h, v_h)|}{\|v_h\|_V} \ge \frac{|b(u_h, Tu_h)|}{\|Tu_h\|_V} = \sup_{v \in V} \frac{|b(u_h, v)|}{\|v\|_V} \ge \gamma \|u_h\|_U,$$
(1.19)

so, we have inf-sup constant $\gamma_h \ge \gamma$.

Theorem 1

The trial to test operator $T: U \longrightarrow V$ is defined by:

$$Tu = R_V^{-1} Bu, \quad u \in U, \tag{1.20}$$

where $R_V : V \longrightarrow V'$ is the Riesz operator corresponding to test inner product. In particular, T is indeed linear.

It can be shown ([21]) that the Ideal Petrov-Galerkin method introduced above is equivalent to a mixed-method as well as a minimum residual method where residual is defined in a dual norm. The ideal PG method benefits from a built-in error indicator for mesh adaptivity thanks to the corresponding mixed method where Riesz's representation of the residual in the dual test norm has been exploited. Assume ϵ is the solution of the following variational form for a given $u_h \in U_h$:

$$(\epsilon, v)_V = l(v) - b(u_h, v), \quad \forall v \in V,$$
(1.21)

the Riesz representation of the residual ϵ is uniquely defined by (1.21). Then the following mixed problem can be defined

$$u_{h} \in U_{h}, \quad \epsilon \in V,$$

$$(\epsilon, v)_{V} + b(u_{h}, v) = l(v), \quad v \in V,$$

$$b(\delta u_{h}, \epsilon) = 0, \quad \delta u_{h} \in U_{h},$$

$$(1.22)$$

where the solution of the Ideal Petrov-Galerkin problem with optimal test space can be derived from solving the mixed Galerkin problem (1.22). It is worth noticing that the method inherently has a built-in residual a-posteriori error ϵ measured in the test norm.

Nevertheless, determining the optimal test functions analytically except for some simple model problems is impossible. Therefore, to some extent approximating optimal test space in a way that discrete inf-sup condition satisfies, is a necessity. An enriched test subspace $V_h \subset V$ is exploited as a remedy for this approximation. So, the Practical Petrov-Galerkin method with optimal test space approximated by enriched test space can be obtained as follows:

$$\begin{cases} u_h^r \in U_h, \\ b(u_h^r, T^r \delta u_h) = l(T^r \delta u_h), \quad \delta u_h \in U_h, \end{cases}$$
(1.23)

where approximated optimal test space computes with component satisfy the standard discretization

$$\begin{cases} T^{r} u \in V^{r}, \\ (T^{r} u, \delta u_{h})_{V} = b(u, \delta v), \quad \delta v \in V_{r}. \end{cases}$$
(1.24)

Indeed, we increase the dimension of the discrete enriched test space to meet the discrete inf-sup condition for the system (1.15). this strategy is valid due to the Brezzi's theory [21] that allows the dimension of discrete test space V^r exceed the dimension of the trial space despite Babuška's theory which enforces the dimension of discrete trial and dimension of discrete test space to overlap. Analysis of stability reduction in the practical Petrov-Galerkin method can be performed by exploiting Fortin operators.

In spite of the myriad of advantages that the practical Petrov-Galerkin Method introduced so far enjoys, due to computation of optimal test space globally through operator T, it is very expensive. Utilizing a broken test space overcomes the issue with localizing evaluation of optimal test space that is conforming element-wise. Therefore, using the method with discontinuous optimal test space will parallelize the assembly of the computation alongside the local computation of test space making the method reliable and viable. Besides, this will justify the name of the Discontinuous Petrov-Galerkin method (DPG) with optimal test functions. However, breaking the test space will bring the need for introducing additional trace variables and flux variables on the mesh skeleton on the element interface.

1.4 Functional Spaces and Preliminaries

In this Dissertation, we assume V is an infinite-dimensional function space where the weak formulation of equation (1.13) is defined, and it has the following form:

$$V := H^{1}(\Omega) = \left\{ u \in L^{2}(\Omega) \mid \frac{\partial u}{\partial x} \in L^{2}(\Omega) \right\},$$
(1.25)

where Ω is the spatial domain of the problem such that in one-dimension the truncated domain is $[x_{\min}, x_{\max}]$, and $L^2(\Omega)$ is the Hilbert space of square integrable with the inner product (\cdot, \cdot) defined as follows:

$$(u,v) := \int_{\Omega} uv dx, \tag{1.26}$$

with the induced norm $||u||_{L^2(\Omega)} = (u, u)^{\frac{1}{2}}$. In the process of designing the finite element method to solve the weak formulation defined in the next section, infinite-dimension space *V* is approximated by the space of continuous piecewise function V_h on an element of Ω which is a finite dimension space. Indeed, functional space defined in (1.25) is a Sobolev space endowed with the norm

$$\|u\|_{H^{1}} = \left(\|u\|_{L^{2}(\Omega)}^{2} + \|\frac{\partial u}{\partial x}\|_{L^{2}(\Omega)}^{2}\right)^{\frac{1}{2}},$$
(1.27)

and semi-norm $|u|_{H^1}$ as follows:

$$|u|_{H^1} = \left(\left\| \frac{\partial u}{\partial x} \right\|_{L^2(\Omega)}^2 \right)^{\frac{1}{2}}, \qquad (1.28)$$

accordingly, $H_0^1 = H_0^1(\Omega)$ is the Sobolev space $H^1(\Omega)$ that vanishes outside of a compact support on $\partial\Omega$ boundary of the domain. However, we are using $\|.\|_r$ for norm of sobolev space of $H^r(\Omega)$ which one can find a detailed definition in [12].

CHAPTER II

VARIATIONAL INEQUALITIES AND SOLUTION APPROACHES

This chapter discusses the different forms of variational inequalities and their corresponding solution approaches with the objective to create a unified path dependence sensitivity analysis formulation of elasto-plastic problem. The different forms include the complementarity problem, optimization problem, fixed-point problem and the Weiner-Hopf equation. The solution of a prototype plasticity problem is presented based on the projection approach and semi-smooth analysis. Path dependent sensitivity analysis of the same problem is performed on the corresponding primal formulation. The solution of a variational inequality arising from a one-dimensional prototype contact problem and semi-smooth solution and sensitivity analysis of one dimensional plasticity problem with linear hardening is presented using Galerkin discretization to demonstrate computational efficiency and accuracy of the discussed theoretical aspects.

2.1 Introduction

Variational inequality is a broad class of problems and is studied in continuum mechanics in the form of plasticity and contact mechanics. Return mapping algorithm is a general and probably the most popular algorithm for solving plasticity problems[79]. The problem of perfect plastic material was first considered by Duvant and Lion[24]. They studied the partial differential equation of elastoplasticity problem. Johnson[47] developed the theorems for existence of plasticity problems, and used variational inequalities to compute solution. The numerical approximation of variational inequality and their corresponding related problems has dramatically increased in the recent years. Weimin and Reddy[34] studied two alternative variational formulation as the primal and dual problems. They defined the primal problem based on a dissipation function, which is a widely used kinematic (displacement-based) formulation. Whereas, the formulation based on yield function is used to define the corresponding dual problem. Gao[31] showed that dual version is an easier approach in non-smooth equilibrium problems. Linear Complementarity problem was used by Stamacchia and Guido[88] in order to solve the quadratic programming problem obtained from Galerkin approximation. Gerhard[81] borrowed the primal-dual interior point method from convex programming to solve the small-deformation, rate-independent elastoplastic response using finite element methods. Krabbenhoft[50] developed a new method based on the second-order cone and semi-definite programming for solution of cam clay plasticity. This new scheme was far more accurate in comparison with the conventional methods where the material point is used to integrate the constitutive equations and a Newton-Raphson like scheme is used to minimize the out-of-balance forces on the structure. However, the Newton-Raphson solver used in this scheme required more iterations than the conventional method. Discrete variational inequality was studied by Weiners and Wohlmuth[?]. Indeed, they showed that using the classical return mapping algorithm for inequality is equivalent to a semi-smooth Newton method for the nonlinear system of equations.

Adaptive methodology based on the finite element method[72, 82, 29, 32] is developed in the hope of analyzing and approximating the solution of elastoplastic problems. Rannacher and Suttmeier[72] benefit from controlling the error obtained from the adjoint solution as a feedback filtering to

yield optimal meshes in linear elasticity. Suttmeier[82] proposed a unified framework for refining meshes based on the concept of a-posteriori error estimation and adaptive mesh design for finite element models of variational inequalities in contact problems. Bangerth and his colleagues[29] applied a set of methods for solving large-scale elastoplastic contact problems with hardening. They used active set method for the contact problems, adaptive finite element discretization with linear and quadratic elements as well as a Newton linearization of the plasticity problem to develop an efficient method. In 2016 Ghorashi and Rabczuk[32] developed a goal-oriented error estimation methodology to estimate the solution of three dimensional elastoplastic problem.

There are some classical examples of variational inequalities such as Strang's problems, contact or obstacle problems[83]. Strang's problem is a problem from elasto-plasticity theory in which the imposed constraints are nonlinear. A fundamental model of contact problem in elasticity is Signorini's problem. Mathematical programming has been used as an effective tool in the development of variational inequalities. It has been used by researchers in the field to not only study the existence, uniqueness and properties of the solution, but also to efficiently approximate solution of variational inequalities.

Sensitivity analysis of variational inequality and nonlinear complementarity problem has been broadly investigated for special forms and under specific theoretical assumptions, but one could barely find a unified sensitivity analysis which satisfies both computational and analytical demands. Former studies of sensitivity analysis was performed as a result of Robinson's[75, 76] finding on generalized equations. Sensitivity of variational inequality has been studied by researchers such as Dafermos [15], Harker [36, 37], Kyparisis [52, 54], and Pang [54] and the references therein. Likwise, sensitivity of nonlinear complementarity problem has been developed by authors like Doung [33], Kojima [48], Miller [65], McLinden [62], Megiddo [64], Pang [54], and Robinson [75], [76]. In addition, sensitivity analysis has been studied for special forms of variational inequality. Kyparisis[53] studied finite dimensional variational inequality and nonlinear complementarity problem thanks to Robinson's results. Investigation on perturbed quasi variational inequality was conducted by Noor[69]. Although, there are authors, such as Dafermos[15], who track the sensitivity analysis of variational inequality from a path which was totally different from Robinson's finding. Indeed, Dafermos tried to solve the problem based on direct geometric arguments. It is worth noticing that the aforementioned papers include the existence and uniqueness of perturbed problem of either variational inequality or nonlinear complementarity problem and they suffer form lack of clear computational algorithms and strategies.

Topological sensitivity of problems pertaining to variational inequality has been investigated over the last decade. Hintermüller[38, 42] studied the abstract shape and topology optimization of elliptic and semi-linear variational inequality. However, among variant problems that lead us to a variational inequality, using inelastic material models brings path-dependency into the model which turns computing of design sensitivity to a nontrivial task. Indeed, this complexity is raised due to the fact that material state depend on the whole history of deformation. Alberdi [?] and his colleges developed a unified framework for adjoint sensitivity of problem involving inelastic materials based on the return mapping algorithm.

In this paper, first we present a brief review of variational inequalities and interconnected problems like quadratic programming problem, complementarity problems, fixed-point problem and Wiener-Hopf equation. Approximating the variational inequality using a finite element space, we present the finite dimensional variational inequalities and related problems. Besides, a prototype plasticity problem with linear hardening as an application of variational inequalities is investigated through semi-smooth analysis. Indeed, using the projection approach, the mixed variational inequality of plasticity problem reduces to a primal problem, and formal linearization paves our way to use iterative method such as generalized Newton's method to find the solution of primal problem including non-differentiable projection. In addition, adjoint and direct path-dependence sensitivity of plasticity problem is developed thanks to the same linearization.

The structure of this chapter is as follows: In Section 2.2, we present the standard form of variational inequality and related problems. Finite element approximation of variational inequalities is explained in Section 2.3. Finite dimensional variational inequality and equivalent problems are developed in Section 2.3.1. Besides, in this Section, we provide numerical solution of one dimension contact problem with the quadratic programming approach and complementarity problem approach based on finite element approximation. Section 2.5 provides semi-smooth analysis of a prototype plasticity problem. Sensitivity analysis of the prototype plasticity problem are discussed in section 2.5.1. Then semi-smooth analysis of solution of one dimensional prototype plasticity problem is performed. Finally, computational results for sensitivity analysis of plasticity problem uses to illustrate the efficiency of proposed sensitivity analysis in the section 2.5.1.

2.2 Variational Inequalities and Related Problems

In this part, we review the related problems of variational inequalities. The material is partly taken from the references by Glonowski[60] and Noor[69]. Let H be a real Hilbert space with the associated inner product and norm denoted by $\langle \cdot, \cdot \rangle$ and $\|.\|$, respectively, and *K* be a closed nonempty convex set in H. We consider the minimization of the following functional

$$I[v] = \langle Tv, v \rangle - 2\langle f, v \rangle \quad \forall v \in H,$$

$$(2.1)$$

where $f : H \to R$ is a linear continuous functional on H and $T : H \to H$ is a continuous operator. This functional is named as the potential (energy, cost) functional. If the operator *T* is linear, symmetric and positive, one can show that the problem of finding minimum of Eq. (2.1) is equivalent to finding *u* satisfying the following problem

$$\langle Tu, v - u \rangle \ge \langle f, v - u \rangle \quad \forall v \in K.$$
 (2.2)

■.

this problem is know as a variational inequality which was introduced and studied by Stampacchia[80] and Fichera[28] in 1964.

Theorem 2

If T is linear, symmetric and positive operator on H, then the variational inequality of Eq. (2.2) is equivalent to the quadratic programming of Eq. (2.1)

Proof: see [28].

The quasi-variational inequality is the variational inequality in which the convex set K depends on the solution of the problem. One example of this case is Signorini's problem. Indeed, a quasi variational inequality is the problem of finding $u \in K(u)$ such that

$$\langle Tu, v - u \rangle \ge \langle f, v - u \rangle \quad \forall v \in K(u),$$
(2.3)

where for any element of *H*, *K*(*u*) is a closed convex subset of *H*. Now, assume that $K^* = \{u \in H : (u, v) \ge 0, \forall v \in K\}$ is the polar cone of the convex *K* in *H*. Problem of finding *u* such that

$$u \in K$$
, $(Tu - f) \in K^*$ and $\langle Tu - f, u \rangle = 0$ (2.4)

is called the Generalized Complementarity problem. Theorem 3 shows that problem of equation (2.2) is equivalent to the problem of Generalized complementarity problem.

Theorem 3

If K^* is the polar cone of the convex set K of Hilbert space H, then the Generalized Complementarity problem Eq. (2.4) is equivalent to Eq (2.2).

Proof: see [69].

Similarly, this problem as well as the above theorem can be modified for a quasi variational inequality. We present some standard results that are basis of many algorithms for solution of variational inequalities. For more detailed properties and proofs one can see[69, 9, 60] and references therein.

Lemma 1

Let K be a closed convex set in H. Then, for a given $z \in H$, $u \in K$ satisfies

$$\langle u - z, w - u \rangle \ge 0 \quad \forall w \in K,$$

$$(2.5)$$

if and only if

$$u = P_K z, \tag{2.6}$$

Proof: see [69].

Using constructive proofs for existence and uniqueness of the solution of variational inequalities, they bring approximation and theory of these problems together[69, 9, 60]. In fact, many numerical algorithms used to show the existence of the solutions are used in the computational area[60] and references therein. Now, we mention the equivalence of variational inequalities and fixed-point problem. Theory and application of this relation can be found in[?, 73, 23, 74, 60]. This equivalence has been used to introduce and develop new algorithm to approximate the solution of variational inequalities[60, 83, 82]. The following well-known results play an important role in developing numerical algorithm.

Theorem 4

The function $u \in K$ is a solution of the variational inequality (2.2), if and only if $u \in K$ satisfies the relation

$$u = P_K[u - \rho(Tu - f)] \tag{2.7}$$

where $\rho > 0$ is a constant and P_K is the projection of H into K.

Proof: see [60].

Eq. (2.7) represents the fixed-point problem which has been exploited for finding solution of variational inequality both theoretically and numerically. Indeed, this projection is the basis of iterative methods such as PSSOR and Uzawa algorithm[79, 82, 60]. The generalized Wiener-Hopf equation is the following equation

$$TP_{K}v + \rho^{-1}Q(v) = f$$
(2.8)

where $Q = I - P_K$ and $T : H \to H$ be a continuous nonlinear operator. Due to the theorem 4 and lemma 1, one can show that there is an equivalence between solution of generalized Wiener-Hopf equation and a variational inequality.

Theorem 5

The variational inequality Eq. (2.2) *has a solution u if and only if the Wiener-Hopf equation* (2.8) *has a solution u, where*

$$v = u - \rho(Tu - f)u \tag{2.9}$$

and

$$u = P_K v \tag{2.10}$$

Proof: see [82].

Theorem 6

For a given linear continuous functional f on H, the variational inequality problem (2.2) has a unique solution if and only if the Wiener-Hopf equation (2.8) has a unique solution.

Proof: see [82].

Results stated showed that three form of problems are equivalent. Indeed, this plays an important role to analyze and develop various numerical algorithm to approximate the solution of the variational inequalities. One can find the summary of this section for variational inequalities, related problems and associated theorems in Figure 2.1.

2.3 Finite Element Approximation of Variational Inequalities

We use the Galerkin finite element approximation of N_h triangular, quadrilateral or hexahedral elements τ_i , satisfying the usual condition of shape regularity, on $T_h = {\tau_i | 1 \le i \ge N_h}$ decom-


Figure 2.1: Variational Inequality and Related Problems

position of Ω . $u_h \in K_h$ is the approximation of the solution $u \in K$ of Eq. (2.2) satisfying the following equation

$$\langle Tu_h, v_h - u_h \rangle \ge \langle f_h, v_h - u_h \rangle \quad \forall v_h \in K_h,$$
 (2.11)

where H_h is the finite elements space on the T_h decomposition and the $K_h \subseteq H_h$ is the appropriate subset of FE-space. Glonowski[60] showed (Theorem (2)) that Eq. (2.11) has a unique solution.

In this chapter, we use the formulations mentioned above to approximate the continuous form of variational inequality and related problems. In fact, using this approximation, we transfer an infinite dimensional problem to a finite dimensional problem. Variational inequality and related problems in finite dimensions are presented in the next section.

2.3.1 Finite dimensional Variational Inequality and Related Problems

First we introduce the finite dimension variational inequality which is similar to Eq (2.11). Assume that matrix $M \in \mathbb{R}^{m \times m}$, vectors $g = (g_1, g_2, \dots, g_m) \in \mathbb{R}^m$ and $q \in \mathbb{R}^m$ are given. Problem of finding $y \in K = \{(x_1, x_2, \dots, x_m) : x_i \ge g_i\}$ such that

$$(My+q, w-y) \ge 0, \quad \forall w \in K$$

$$(2.12)$$

is a finite dimensional variational inequality. One can easily show that Eq. (2.12) corresponds to the following finite dimensional constraint optimization problem

$$\begin{cases} \min(My+q, y) \\ s.t \quad y \in K \end{cases}$$
(2.13)

It can be shown that solution of problem (2.12) satisfies the solution of (2.13) and vice-a-versa. Another related problem that is mentioned in the Section 2.2 is a fixed-point problem or generalized Wiener-Hopf equation. Considering Lemma (1) and Theorem (4) one can define the corresponding fixed-point problem (or Wiener-Hopf equation) as

$$y = P_K(y - (My + q))$$
 (2.14)

where P_k is the projection of space \mathbb{R}^m into K. However, problem of finding explicit form of this projection in a general form is a tedious task. Nevertheless, we introduce the explicit form of this projection for the plasticity problem with hardening in next section. Considering theorem (2) and the fact that when convex cone K is the non-negative orthant of \mathbb{R}^m , the dual cone K^* is the same space as convex cone *K*, the equivalent complementarity problem (CP) can be define as finding $y \in \mathbb{R}^m$ such that

$$\begin{aligned}
 &My + q \ge 0, \\
 &y - g \ge 0, \\
 &(y - g)^T (My + q) = 0.
 \end{aligned}$$
(2.15)

Besides, standard form of complementarity problem is obtained by the change of variables b = Mg + q, x = y - g, and is written as

$$\begin{cases} x \ge 0, \\ Mx + b \ge 0, \\ x^{T}(Mx + b) = 0. \end{cases}$$
 (2.16)

Different direct and iterative algorithms have been developed to solve the standard (CP) Eq. (2.16) such as family of active set methods as direct algorithms and generalized Newton's method (or so-called semi-smooth Newton's method) [83, 42, 41, 18]. In fact, family of Newton's method has been shown to be the fastest algorithm [18]. In the next section, we exploit general form of semi-smooth Newton's approach for the solution of a non-differentiable variational equation obtained from a mixed variational inequality.

2.4 A Prototype Contact Problem

The fundamental model for contact problem, called Signorini's problem is written in classical form as[60, 70]

$$-\operatorname{div} \sigma = f, \quad A\sigma = \epsilon(u) \quad \text{in} \quad \Omega$$

$$u = 0 \quad \text{on} \quad \Gamma_D$$

$$\sigma \cdot n = t \quad \text{on} \quad \Gamma_N$$

$$\sigma_T = 0, \quad (u_n - g) \cdot \sigma_n = 0 \quad \text{on} \quad \Gamma_C$$

$$u_n - g \le 0, \quad \sigma \le 0 \quad \text{on} \quad \Gamma_C$$

$$(2.17)$$

The deformation of an elastic body using the domain $\Omega \subseteq \mathbb{R}^d$ is explained with this model. Body force f and traction t along Γ_N can cause the displacement u and the corresponding stress tensor σ . $\Gamma_C \subseteq \partial \Omega$ is a possible contact surface and body is fixed through the Dirichlet condition on Γ_D . The simplified form of this problem in one-dimension is as following

$$-\Delta u = f \quad \text{in} \quad \Omega \subset \mathbb{R}$$

$$u = 0 \quad \text{on} \quad \Gamma_D,$$

$$u \ge 0, \quad \partial_n u \ge 0, \quad u \partial_n u = 0 \quad \text{on} \quad \Gamma_C$$
(2.18)

where $\Gamma_C = \partial \Omega \setminus \Gamma_D$ and $\partial_n u = \nabla u \cdot n$. The corresponding form of Eq. (2.18) as a variational inequality reads

$$(\Delta u, \Delta(\phi - u)) \ge (f, \phi - u) \quad \forall \phi \in K$$
(2.19)

where $V = \{v \in H^1 : v = 0 \text{ on } \Gamma_D\}$ and $K = \{v \in V : v \ge 0 \text{ on } \Gamma_C\}$.

In this Section we use convex optimization techniques and complementarity problem approach based on Galerkin finite element approximation to compute the solution of Eq. (2.19) in a one dimensional case. The prototype problem Eq. (2.19) is presented to illustrate the finite element approximation. This example is a one dimensional contact problem where the obstacle function is in contact with the solution. In this example the domain $\Omega = [0, 1]$, and the obstacle function is a piecwise constant function. The contact problem is as following

$$-k\frac{d^{2}u}{dx^{2}} = f \quad \text{on} \quad \Omega = [0, 1]$$
$$u(0) = u(1) = 0 \tag{2.20}$$
$$u(x) \le \Psi(x) \quad x \in \Omega_{c}$$

Where the solution is in contact with the obstacle function $\Psi(x)$ on Γ_c . We define $\Psi : \Omega \to R$ as a constant function $\Psi(x) = c$ on interval $\Omega_c = [0.4, 0.6]$ and zero for $\Omega \setminus \Omega_c$. However when derivative of the solution has contact with obstacle function we can use the same techniques with a modification on the convex cone. Using the fact that the solution of variational inequality with the symmetric bi-linear form is equivalent to the minimization of corresponding energy function, we used finite element to approximate the solution of optimization problem. Computation is realized in Matlab through the fmincon. In addition, semi-smooth Newton's method is performed for solving the corresponding complementarity problem through PETSc library[18] in C + +. The corresponding variational inequality form of Eq. 2.20 reads

$$\left(\frac{d\phi}{dx}, k\frac{du}{dx}\right) \le (\phi, f) \quad \text{on} \quad K$$

$$(2.21)$$

$$K = \{u \in C^{1}(\Omega) | \quad u(x) \le \Psi(x)\}$$

The results from section 2.2 implies that the solution of Eq. (2.21) can be obtained from the following optimization problem

$$\min_{u \in K} \int_{\Omega} \left(\frac{1}{2} \left(k \frac{du}{dx} \right)^2 - u.f \right) d\Omega$$
(2.22)

where the minimization is performed on convex subset of $C^1(\Omega)$ defined in Eq. (2.21). Besides, we know from section 2.2, Theorem. 5, the solution of this contact problem can be computed from the corresponding complementarity problem which reads

$$(-u(x) + \psi(x)) \ge 0, \quad (-k\frac{d^2u}{dx^2} - f) \ge 0, \quad \langle -u(x) + \psi(x), -k\frac{d^2u}{dx^2} - f \rangle = 0$$
 (2.23)

where $\langle \cdot, \cdot \rangle$ is the inner-product in *R*. As we discussed in section 2.3.1 there are different methods which can be used to approximate the solution of this complementarity problem. we used semismooth Newton's method to deal with the solution of Eq. (2.23). Figure (2), (3) depicts the solution of contact problem with optimization approach and complementarity problem approach respectively for two different values of c = 0.08, 0.18.

It is worth noticing that the contact problem in which the derivative of solution is bounded by a obstacle function $K = \{u \in C^1(\Omega) | |\frac{\partial u}{\partial x}| \le \psi(x)\}$ could be converted to a corresponding optimization and complementarity problems.

2.5 A Prototype Problem in Plasticity

It is well-known that materials exhibit plastic strain when internal stresses exceed a limit condition. This special change in behaviour of deformation is called elastoplasticity. In this



Figure 2.4: The approximate solution of the optimization form of the one dimensional variational inequality for two different obstacle functions.



Figure 2.7: The approximate solution of the equivalent complementarity problem form of the one dimensional variational inequality for two different obstacle functions.

section, we study mathematical model of this behaviour with linear hardening. [47, 84] This problem is formulated as partial differential equation constrained with inequality stated in the form

of a yield condition. Indeed, internal stress $\sigma(x)$ of plastic materials is limited by a bound that can be expressed by an inequality like

$$\mathcal{F}(\sigma) \le 0 \tag{2.24}$$

One choice for \mathcal{F} is the von Mises flow function $\mathcal{F}(\sigma) = \|\sigma^D\| - \sigma_y$, where σ_y is the yield stress, and $\sigma^D = \sigma - \frac{1}{3} \operatorname{trace}(\sigma) I$ is deviatoric part of stress tensor. This special form of \mathcal{F} is considered as a simplest example. Due to the inequality in Eq. (2.24) the elastoplastic problem is expressed as a variational inequality. In the following we study a prototype mathematical model which is conceptually connected to the elasticity problem. The prototype problem of elastoplasticity with linear hardening reads [84, 29]

$$-k \operatorname{div} \sigma = f, \quad \sigma = \prod_{\xi} \nabla u \quad \text{in} \quad \Omega, \quad u = 0 \quad \text{on} \quad \partial \Omega$$
 (2.25)

which seeks *u* and flux vector $\sigma = (\sigma_1, \sigma_2)$. The plastic behaviour of material is restricted by a nonlinear function $\mathcal{F}(\sigma, \xi) = \sqrt{\|\sigma : A : \sigma\|} - (\alpha \xi + \sigma_y) \le 0$, where *A* is a symmetric second order tensor, $\alpha > 0$, $\xi = \xi(\nabla u)$ and for the rest of his paper we assume $\sigma_y = 1$. Π_{ξ} is the projection to yield surface. Now, we need to define the following spaces and notations in the hope of introducing the weak form

$$V = \{ u \in H^1(\Omega) : u = 0 \text{ on } \Gamma_u \},$$

$$(2.26)$$

$$L^{2}(\Omega)^{2} := L^{2}(\Omega, \mathbb{R}^{2}),$$
 (2.27)

$$\Pi H = \{(\tau, \eta) \in L^2(\Omega)^2 \times L^2(\Omega)^2) : \mathcal{F}(\tau, \eta) \le 0\},$$
(2.28)

$$\mathcal{F}(\sigma, \alpha) = \sqrt{\|\sigma : A : \sigma\|} - (\alpha \xi + \sigma_y), \qquad (2.29)$$

The primal-mixed variational formulation of Eq. (2.25) is the problem of seeking a pair $\{u, (\sigma, \xi)\} \in v \times \Pi H$ such that (for more details reader can see [47])

$$(\sigma, \tau - \sigma) + \alpha(\xi, \eta - \xi) - (\nabla u, \tau - \sigma) \ge 0, \quad \forall (\tau, \eta) \in \Pi H$$
(2.30)

$$(k\sigma, \nabla(\phi)) = (f, \phi) \quad \forall \phi \in V$$
 (2.31)

Here (\cdot, \cdot) represents the inner product and Ω a proper bounded domain. If we set $\eta = \xi$ in Eq.(2.30), one can see Lemma (1) that σ is the projection of ∇u onto the yield surface. It is not difficult to see that the projection has the following form

$$\sigma = C(\nabla u) \quad \text{a.e} \quad \text{in} \quad \Omega \tag{2.32}$$

where the projection reads

$$C(\vartheta) := \begin{cases} \vartheta : A : \vartheta, & \text{if } \vartheta : A : \vartheta \le (\alpha \xi + \sigma_y)^2 \\ \sqrt{A^{-1}} (k\alpha + \sigma_y) \frac{\vartheta : A : \vartheta}{|\vartheta : A : \vartheta|} & \text{if } \vartheta : A : \vartheta > (\alpha \xi + \sigma_y)^2 \end{cases}$$
(2.33)

where square root of tensor is defined through spectral decomposition of tensor A. Furthermore, we have the following relations [47],

$$\xi = \beta(|\nabla u| - 1), \quad \beta = -\frac{1}{1 - \alpha^2}(\alpha \pm \sqrt{1 - \alpha^2 + \alpha^4})$$
 (2.34)

substituting Eq. (2.34) and Eq. (2.32) into Eq. (2.31), one can obtain the following nonlinear variational equation

$$(kC(\nabla u), \nabla(\phi)) = (f, \phi) \quad \forall \phi \in V$$
(2.35)

The approximate solution of (2.35) is determined by the discrete equation

$$(kC(\nabla u_h), \nabla(\phi)) = (f_h, \phi) \quad \forall \phi \in V_h$$

$$(2.36)$$

$$33$$

where corresponding finite element space is shown by notation $V_h \subset V = H_0^1(\Omega)$. Iterative algorithm is a common technique for the solution (2.36) such as Newton's method. However, since the projection $C(\nabla u)$ is not differentiable, one should use the general form of Newton's method in the hope of approximating the solution of nonlinear equation

2.5.1 Sensitivity Analysis of Plasticity Problem

In this section, we present the continuum sensitivity approach to attain sensitivity of solution of the plasticity problem stated in the previous Section with respect to the design parameters. The sensitivity analysis is directly performed on the variational formulation of the Eq. (2.35) used for finite element approximation. In the following sections first we study the direct sensitivity and then adjoint sensitivity analysis of the plasticity problem with linear hardening will be presented.

2.5.1.1 Sensitivity of Variational Statement

As we mentioned in the previous section, the variational equation of Eq. (2.35) is the problem of finding *u* such that satisfying the following nonlinear equation

$$(kC(\nabla u), \nabla \phi) = (f, \phi) \quad \forall \phi \in V$$
(2.37)

where ϕ is an arbitrary variation belonging to the proper space. The sensitivity analysis of this variational form reads

$$((kC(\nabla u))_{\alpha}, \nabla(\phi)) + ((kC(\nabla u), \nabla\phi_{\alpha}) - (f_{\alpha}, \phi) - (f, \phi_{\alpha}) = 0 \quad \forall \phi \in V$$
(2.38)

where $(\cdot)_{\alpha} = \frac{d(\cdot)}{d\alpha}$, and as we define ϕ is an arbitrary function in finite element space, ϕ_{α} belongs to the same space as well. Therefore, the second and fourth terms will be equal to zero due to the Eq.

(2.37). Therefore, the sensitivity of variational statement turns to the problem of finding $u_{\alpha} = \frac{du}{d\alpha}$ such that

$$((kC(\nabla u))_{\alpha}, \nabla(\phi)) - (f_{\alpha}, \phi) = 0 \quad \forall \phi \in V$$
(2.39)

It is worth noticing that u_{α} implicitly exists in $C(\nabla u)_{\alpha}$. Thus, solution of nonlinear non-smooth variational equation of Eq. (2.39) will result in u_{α} . In the following Section we define Direct and Adjoint approach to define the sensitivity of response function.

2.5.1.2 Direct Sensitivity

Let $g(\alpha, u)$ is the response functional which is used in the design process, and α is the design parameter. we assume $g(\alpha, u)$ has the following form

$$G = \int_{\Omega} g(\alpha, u) \, d\Omega \tag{2.40}$$

The sensitivity of G with respect to the α is

$$G_{\alpha} = \frac{dG}{d\alpha} = \int_{\Omega} \left(\frac{dg}{d\alpha}(\alpha, u) + \frac{\partial g(\alpha, u)}{\partial u} u_{\alpha} + \frac{\partial g(\alpha, u)}{\partial \xi} \xi_{\alpha} \right) d\Omega$$
(2.41)

Since the nature of plasticity problem is a path-dependent problem, we also need to assess the impact of design parameter α on the internal variable of ξ which is shown by ξ_{α} . When we evaluate the sensitivity of the solution from Eq. (2.39), the sensitivity of *G* can be easily obtained thanks to the equation (2.41).

2.5.1.3 Adjoint Sensitivity

In the direct sensitivity, one should compute the sensitivity of the solution directly. However, adjoint sensitivity does not impose this computational cost to the problem, and it benefits computational efficiency when the number of functionals $g(\alpha, u)$ is greater than the number of parameters

To start, we modified the functional *G* by adding the variational statement and replacing the arbitrary test function ϕ by the adjoint variable λ which is supposed to be zero based on Eq. (2.31). The modified functional is

$$\tilde{G} = \int_{\Omega} g(\alpha, u) \, d\Omega + (kC(\nabla u), \nabla \lambda) - (f, \lambda)$$
(2.42)

The sensitivity of this functional reads

$$\begin{split} \tilde{G}_{\alpha} &= \frac{dG}{d\alpha} = \int_{\Omega} \left(\frac{dg}{d\alpha}(\alpha, u) + \frac{\partial g(\alpha, u)}{\partial u} u_{\alpha} + \frac{\partial g(\alpha, u)}{\partial \xi} \xi_{\alpha} \right) \, d\Omega + \left(k_{\alpha} C(\nabla u), \nabla \lambda \right) + \left(k C_{u}(\nabla u, u_{\alpha}), \nabla \lambda \right) \\ &+ \left(\left(k C(\nabla u), \nabla \lambda_{\alpha} \right) - \left(f_{\alpha}, \lambda \right) - \left(f, \lambda_{\alpha} \right), \end{split}$$

$$(2.43)$$

where u_{α} is the sensitivity of the solution of variational statement Eq. (2.37) with respect to the design parameter α , and λ is adjoint variable from the space of test functions. Now, the forth and sixth term of right hand side will add to zero due to the fact that we assume λ , and λ_{α} to belong to the space of test functions; so, these two terms satisfy a variational form which is zero based on the equation (2.37). Now, we find the adjoint variable λ such that it satisfies

$$\int_{\Omega} \frac{\partial g(\alpha, u)}{\partial u} v \, d\Omega + (kC_u(\nabla u, v), \nabla \lambda) = 0 \quad \forall \quad v \in V.$$
(2.44)

We formed above equation by replacing u_{α} in the second and third term of Eq. (2.43) by an arbitrary variation v and set these two terms to be zero and solution of Eq.(2.44) provides adjoint variable. Finally, the adjoint sensitivity of *G* can be computed as

$$\tilde{G}_{\alpha} = \int_{\Omega} g_{\alpha}(\alpha, u) \ d\Omega + (k_{\alpha}C(\nabla u), \nabla \lambda) - (f_{\alpha}, \lambda)$$
(2.45)

using the adjoint functional λ which satisfies the Eq. (2.44). The advantage of this approach is that we do not need to evaluate the u_{α} .

2.5.2 One-dimensional Prototype Plasticity Problem

In this section, we will provide computational results that support our theoretical finding in one-dimensional case for a prototype plasticity problem with linear hardening. In Section 2.5, we used projection approach to eliminate the plasticity inequality, and turn the mixed variational inequality to a primal problem: Find (u, ξ) in one dimension such that

$$(kC(u',\xi),\phi') - (f,\phi) = 0, \quad \forall \phi \text{ in } V$$
 (2.46)

where $(\cdot)' = \frac{du}{dx}$, with the following projection

$$C(u',\xi) := \begin{cases} u', & \text{if } Au'^2 \le (\alpha\xi + \sigma_y)^2 \\ \sqrt{A^{-1}}(\alpha\xi + \sigma_y)\frac{u'^2}{|u'^2|} & \text{if } Au'^2 > (\alpha\xi + \sigma_y)^2 \end{cases}$$
(2.47)

Our basic approach for approximating the solution of Eq. (2.46) in the finite element space is Newton's method. But, Eq. (2.46) is not formally differentiable. Nevertheless, this nonlinear equation satisfies the slant differentiablity condition. Thus, we will use formal linearization to approximate the solution. In the semi-smooth damped Newton's method we are seeking an update solution $u^{i+1} = u^i - v^i \delta u^i$ where v^i is a damped factor. Using formal linearization, the Newton's step can be obtained using

$$(kC(u^{i\prime},\xi),\phi') - (kC_u(u^{i\prime},\xi;\delta u^i) - (f^i,\phi) = 0, \quad \forall \phi \text{ in } V$$
(2.48)

where $C_u(\cdot, \cdot; \cdot)$ is given by

$$C_{u}(u',\xi;\delta u) := \begin{cases} \delta u', & \text{if } Au'^{2} \leq (\alpha\xi + \sigma_{y})^{2} \\ \left(\frac{\sqrt{A^{-1}(\alpha\beta(|u'|-1)+\sigma_{y})}}{|u'|}(1-\frac{u'}{|u'^{2}|}) + (A^{-1}\alpha\beta)\right)\delta u' & \text{if } Au'^{2} \geq (\alpha\xi + \sigma_{y})^{2} \end{cases}$$
(2.49)

Projection $C(u', \xi)$ introduced in Eq. (2.47) is a function of u' and ξ , but since the ξ depends on u'from Eq. (2.34), we considered $\delta \xi$ implicitly through the linearizaton procedure in direction of δu for both Newton's Method and sensitivity analysis. Note that $C_u(u', \xi; \delta u)$ is a formal linearization of $C(u', \xi)$ around a fixed u' and in the direction δu . If we consider Eq. 2.46 as equation F(u) = 0, one can determined the damped factor v_i as the first real number that fulfills

$$|F(u^{i} - v^{i}\delta u^{i})| < |F(u^{i})|.$$
(2.50)

Figures 4 depicts the quasi-static solution of the one-dimensional plasticity problem and the value of $\xi(x)$ through four loading force steps to reach f = 100. Considering $G = \int_{\Omega} u'^2 d\Omega$ as a



Figure 2.8: Qusi-static solution of the one-dimensional plasticity problem with the hardening parameter $\alpha = 0.1, A = 0.1$, body force f = 25, 50, 75, 100

response function, we study the direct and adjoint sensitivity of solution of plasticity problem with respect to the coefficient k. The sensitivity of variational statement of one dimensional plasticity problem is

$$(C(u'), \nabla\phi) + (kC_u(u', \xi; u_k), \nabla\phi) = \left(\frac{\partial f}{\partial k}, \phi\right) \quad \forall\phi \in V$$
(2.51)

Where $C_k(u', \xi; u_k)$ is the linearization of projection Eq. (2.47) with respect to k. The direct sensitivity of response functional with respect to k obtained from

$$G_k = \frac{dG}{dk} = \int_{\Omega} 2u'u'_k \, d\Omega \tag{2.52}$$

Where $u' = \frac{du}{dx}$ and $u_k = \frac{du}{dk}$. The adjoint sensitivity of response functional with respect to the coefficient *k* include two steps. First, the adjoint variable computes using the following equation

$$\int_{\Omega} 2u'v' \, d\Omega + (kC_u(u',\xi;v),\lambda') = 0, \quad \forall v \in V,$$
(2.53)

where $C_u(\cdot, \cdot; \cdot)$ is the same as linearization we used beforehand, *u* assume to be known as the solutions of Eq. (2.46), (2.51). Using the adjoint functional λ satisfying in Eq. (2.53), one can find adjoint sensitivity of response functional by calculating

$$G_k = \frac{dG}{dk} = (C(u',\xi),\lambda') - (f_k,\lambda).$$
(2.54)

Figure 5 illustrates the direct, adjoint sensitivity and forward finite difference sensitivity of plasticity problem in one dimensional.



Figure 2.9: Sensitivity of response function G

CHAPTER III

A STABLE FINITE ELEMENT ANALYSIS FOR MIGRATION RISK PROBLEM

In this chapter, we propose a finite element method to study the problem of credit rating migration problem narrowed to a free boundary problem. Free boundary indeed separates the high and low rating region for a firm and causes some difficulties including discontinuity of second order derivative of the problem. Exploiting the weak formulation of the problem utilized in the Galerkin method, the discontinuity of second order derivative is averted. In this investigation we prove optimal convergence and stability of the proposed method. Numerical results illustrate how derived convergence results are consistent into practice ones.

3.1 Introduction

Over the recent years, quantitative credit risk modeling of financial institutions has been very popular in academia, industry and among regulators. Indeed, development of financial market of credit securities as well as standards offered by Basel accord have dramatically encouraged this interest. Default event, transition in the credit quality and variation of credit spreads are the main components of the credit risk modeling [10, 63]. Thus, developing efficient and accurate models and measures to identify and quantify credit is a necessity.

However, many investigations correspond credit risk with default risk which is the probability that a counterparty of a financial contract, either issuer of entities or a bank, does not meet the requirement of the contract. We learned the hard way due to the financial crisis that migration risk is also an intrinsic part of credit risk [77, 35]. Credit rating migration indicates that credit quality of a financial institution has upgraded or downgraded. It is well-known that these moves accelerated the eurozone's sovereign debt crisis in 2010 and financial crisis of 2008.

A primary approach for the assessment of credit rating migration in the literature is utilizing the transition matrix of a Markov chain which consists of rating transition probabilities that an obligor migrates up or down to another rating [46, 17]. Former models benefit from the Markov property [46] that assumes that the predicted rating is independent from the rate history, whereas later models have been improved to be more realistic where they are exploiting various items such as the domicile of obligor and business cycle [66, 55, 51], and so forth.

The aforementioned approach is classified as a reduce-form method, which treats the rate migration exogenously without considering structural features of a firm such as asset and debt value of a company which can be essential in migrating a firm's rate.

Some efforts have been made in the literature to broaden Merton method in order to employ the structural models in the purpose of modeling the value of a firm. Liang et al. [58, 59] used a boundary of high rating grade and low rating region obtained form real data using a statistical method as a threshold to determine whether the value of the firm is in a high rate region or a low rate region. The structural model developed with this threshold eventuates in a partial differential equation that has a close form solution under some proper boundary assumptions. However, this threshold is not anticipated in the real world, and later Bei Hu et al. [45] enhanced this model by assuming that the transition threshold is a proportion of structural variables of a firm like its debt and value. This model is then reduced to a free boundary value problem that explains credit rating migration of a firm where the threshold is a free boundary that is implicitly computed through time horizon. Hu and his colleagues in [45] proved that the solution of the derived free boundary problem exists and it is unique. Besides, they showed some regularity properties of the problem including free boundary. Later asymptotic traveling wave solution of a free boundary value problem for the problem of credit rating migration is investigated in [57]. In fact, they showed the existence and uniqueness of the solution of the problem, and using a construction proof benefit from Lyapunov function, they showed that the solution of the free boundary problem is convergent to the traveling wave solution. Yuan Wu et al. [87] studied valuation of a defaultable corporate bond with rating migration under a structural framework where there is a possibility of default apriorily at any time to maturity. They indeed used the first-passage-time model in which a barrier is the predetermined default threshold.

It is now widely known that the free boundary value problem derived from the migration problem, despite the fact of being well-posed, doesn't have a closed form analytical solution. Thus, proposing efficient and accurate numerical methods that approximate the solution as well as the location of the free boundary is necessary. First a comprehensive study in this direction is performed in [56], where authors studied explicit finite difference scheme for numerical remedy of the free boundary problem. The convergence and stability of the method is analyzed in this work, and optimal convergence rate for spatial variable is derived. This finite difference method is proposed for the first time in [45] which corresponds to binomial tree scheme (BTS).

A variety of numerical methods has been exploited to deal with free boundary problems in the field of quantitative finance including finite difference method, finite element method, and recently introduced meshfree methods. However, among aforementioned methods, Galerkin method thanks

to the framework of Hilbert space and Sobolev space is providing a suitable level of abstraction to perform error analysis of proposed schemes. Indeed, monitoring, measuring and controlling the error analysis of the Galerkin method have been broadly and extensively assessed in the field of engineering as well as quantitative finance over a relatively long time. Besides, developing, maintaining, and parallelizing the code for finite element method is trouble free in comparison to finite difference method for instance, and as a result it can lead to stronger and clearer error and convergence analysis. Therefore, we believe that investigating finite element for free boundary problem of migration rate problem is highly advantageous.

Finite element method is utilized to deal with free boundary problems obtained from American option in [2], where the exact discrete free boundary is derived using a stabilized algorithm. Allegretto, Lin and Yang [3] investigated error estimate of finite element method for solving free boundary problem of heat equation obtained by a change of variable in the problem of American option pricing. In fact, they studied the error analysis of variational inequality driven by the problem in a finite region. Holmesa and others in [44, 43] used front fixing finite element method for regime switching and American option with a variational inequality approach. The truncated free boundary value problem is directly computed through solving a nonlinear boundary value problem on a rectangular domain. They also performed the analysis of stability and positivity of the nonlinear system as well. Galerkin method with wavelet basis is used in [61] for dealing with free boundary problems of partial differential equations driven from American option on asset with Lévy price processes. Matche and others [61] benefited from the properties of wavelet basis to precondition the linear system arisen from the corresponding linear complementarity problem (LCP). Kovalov et al [49] used finite element to discretize the nonlinear PDE obtained form

multi-asset American options penalized by a smooth penalty term. They solved the ODE system obtained form the discretization by an adaptive integrator. They also showed that non-smooth penalty improves the efficiency of the adaptive methodology. Furthermore, inverse finite element method is proposed in [89] to solve the nonlinear free boundary problem of American option without any linearization.

In this chapter we develop the Galerkin method for dealing with migration rate problem. First we derive the weak formulation of the free boundary value problem which lessens the regularity requirement for the space of the solution. Since the boundary of the migration region brings discontinuity in the second order derivative, the weak form overcomes this discontinuity. A high order Lagrange finite element space is exploited to approximate the infinite space of the solution by the finite space. Error and stability analysis of the variational form of the parabolic free boundary problem is performed using some theoretical results for the associated elliptic problem. It is worth mentioning that some proofs or results depend on the known results for parabolic problems from the literature [85, 11, 8]. We tackle the free boundary value explicitly using green function and dual problem of the migration problem, and we propose a straight way to find the free boundary as well as the a priori estimation.

Let's briefly review the outline of the remainder of this paper. 3.2 reviews the migration rate problem and presents the approximated system of equations for this problem. In section (3.3), we introduce the function spaces and notations we employ in this paper. Section (3.4) provides the weak formulation corresponding to the migration problem and some elementary properties of the bilinear form. In section (3.5), we ensure that the variational form presented is well-defined and has good regularity properties. Error analysis of approximating the problem in L^2 norm and L_{∞} are presented in section (3.7). Section (3.8) gives stability and convergence analysis of the proposed method. Utilizing green function and adjoint problems corresponding to the credit rating migration problem, an explicit method is proposed to estimate the free boundary. Section (3.10) shows numerical experiments and their results for the proposed method and error analysis.

3.2 Problem of Credit Rating Migration

Credit quality and default probability of a corporation is gauged by the bond rating. In this section, we review the structural model to value the bond so as to assess the problem of credit rating migration. Let's assume that the firm issues solely a single zero-coupon bond with the face value *K* which has a discount value of Φ_t at time *t*. Let (Ω, \mathcal{F}, P) be a complete probability space, and W_t is the Brownian motion adapted to the filtration of \mathcal{F} , the value of firm in the neutral world denoted by S_t satisfies the following system:

$$dS_t = \begin{cases} rS_t dt + \sigma_H S_t dW_t, & S_t \in \Omega_H, \\ \\ rS_t dt + \sigma_L S_t dW_t, & S_t \in \Omega_L, \end{cases}$$
(3.1)

where *r* is the risk free interest rate, and the volatilities $\sigma_H < \sigma_L$ show the volatility of the firm in two regimes of low and high credit grades where high rating region and low rating region are shown by Ω_H and Ω_L respectively. Up region and low region are decided by the proportion of the debt and value of the firm with a threshold boundary which is represented by the constant 0 < v < 1. Besides, it is trivial that if the maturity of the bound is in time *T*, the gain of an investor can be $\Phi_T = \min\{S_T, K\}$ depending on the insolvency of the firm. One can show [6, 22] that $V_H(S_t, t)$ and $V_L(S_t, t)$ the values of bond in up and down grades with respect to the value of firm S_t at time t satisfy the following system of PDEs with free boundary

$$\begin{cases} \frac{\partial V_H}{\partial t} + \frac{1}{2}\sigma_H^2 S^2 \frac{\partial^2 V_H}{\partial S^2} + rS \frac{\partial V_H}{\partial S} - rV_H = 0, \quad S > \frac{1}{\nu} V_H, \quad t > 0, \\ \frac{\partial V_L}{\partial t} + \frac{1}{2}\sigma_L^2 S^2 \frac{\partial^2 V_L}{\partial S^2} + rS \frac{\partial V_L}{\partial S} - rV_L = 0, \quad 0 < S < \frac{1}{\nu} V_L, \quad t > 0, \\ V_H(S,T) = V_L(S,T) = \min\{S,K\}, \end{cases}$$
(3.2)
$$\frac{\partial V_H}{\partial S}(s_f,t) = \frac{\partial V_L}{\partial S}(s_f,t), \quad s_f : \text{rating migration boundary} \\ V_H(s_f,t) = V_L(s_f,t), \quad s_f : \text{rating migration boundary} \end{cases}$$

Using the standard change of variable $v(x, t) = V_H(e^x, T - t)$ in high rating region and $v(x, t) = V_L(e^x, T - t)$ in low rating region, switching to $x = \log \frac{S}{K}$, renaming T - t = t, and assuming without losing generality that the face value K = 1, the following system of free boundary problems will be obtained

$$\begin{cases} \frac{\partial v}{\partial t} - \frac{1}{2}\sigma_{H}^{2}\frac{\partial^{2}v}{\partial S^{2}} - (r - \frac{1}{2}\sigma_{H}^{2})\frac{\partial v}{\partial S} - rv = 0, \quad v < ve^{x}, \quad t > 0, \\\\ \frac{\partial v}{\partial t} - \frac{1}{2}\sigma_{L}^{2}\frac{\partial^{2}v}{\partial S^{2}} - (r - \frac{1}{2}\sigma_{L}^{2})\frac{\partial v}{\partial S} - rv = 0, \quad v \ge ve^{x}, \quad t > 0, \end{cases}$$

$$(3.3)$$

$$v(x, 0) = \min\{S, 1\}, \\\\ \lim_{x \to s_{f}^{-}} \frac{\partial v}{\partial S}(x, t) = \lim_{x \to (s_{f})^{+}} \frac{\partial v}{\partial S}(x, t), \\\\ \lim_{x \to s_{f}^{-}} v(x, t) = \lim_{x \to s_{f}^{+}} v(x, t) = ve^{s_{f}}. \end{cases}$$

Now, if we rewrite the volatilities in high and low rating regions as $\sigma = \sigma_H + (\sigma_L - \sigma_H)H(v - ve^x)$, where H(x) is the Heaviside function, the following approximated system can be defined [45]

$$\begin{cases} \frac{\partial v_{\epsilon}}{\partial t} + \mathcal{L}v_{\epsilon} = 0 \quad x \in \mathbb{R}, \quad 0 < t \le T, \\ v_{\epsilon}(x, 0) = G(x), \quad x \in \mathbb{R}, \end{cases}$$

$$\sigma_{\epsilon}(v_{\epsilon}(x, t), t) = \sigma_{H} + (\sigma_{L} - \sigma_{H})H_{\epsilon}(v_{\epsilon}(x, t) - ve^{-\delta t}) \end{cases}$$
(3.4)

in which the elliptic operator $\mathcal{L}v_{\epsilon}$ represents the following:

$$\mathcal{L}v_{\epsilon} = -\frac{1}{2}\sigma_{\epsilon}^{2}(v_{\epsilon}(x,t),t)\frac{\partial^{2}v_{\epsilon}}{\partial x^{2}} - \left(r + \frac{1}{2}\sigma_{\epsilon}^{2}(v_{\epsilon}(x,t),t)\right)\frac{\partial v_{\epsilon}}{\partial x},$$
(3.5)

the function $G(x) = \min\{1, e^x\}$, and H_{ϵ} is a C^{∞} function that approximates the Heaviside function (see [45] for more details), defined as follows:

$$\begin{cases}
H_{\epsilon}(x) = 0, \quad x \leq -\epsilon \\
H_{\epsilon}(x) = 1, \quad x \geq 0,
\end{cases}$$
(3.6)

such that this function has these properties

$$0 \leq H_{\epsilon}'(x) \leq C \epsilon^{-1}, \quad |H_{\epsilon}''(x)| \leq C \epsilon^{-2}.$$

The equation (3.4) has a unique solution [6] for every $\epsilon > 0$. However, designing an efficient numerical solution of this equation due to the fact that the analytical solution is not available in hand is essential. In the proceeding sections, the proposed method to solve this free boundary value problem is presented.

3.3 Functional Spaces and Preliminaries

In this paper we assume V is an infinite-dimensional function space where the weak formulation of equation (3.2) is defined, and it has the following form:

$$V := H^{1}(\Omega) = \left\{ u \in L^{2}(\Omega) \mid \frac{\partial u}{\partial x} \in L^{2}(\Omega) \right\},$$
(3.7)

where Ω is the spatial domain of the problem such that in one-dimension the truncated domain is $[x_{\min}, x_{\max}]$, and $L^2(\Omega)$ is the Hilbert space of square integrable with the inner product (\cdot, \cdot) defined as follows:

$$(u,v) := \int_{\Omega} uv dx, \tag{3.8}$$

with the induced norm $||u||_{L^2(\Omega)} = (u, u)^{\frac{1}{2}}$. In the process of designing the finite element method to solve the weak formulation defined in the next section, infinite-dimension space *V* is approximated

by the space of continuous piecewise function V_h on an element of Ω which is a finite dimension space. Indeed, functional space defined in (3.7) is a Sobolev space endowed with the norm

$$\|u\|_{H^{1}} = \left(\|u\|_{L^{2}(\Omega)}^{2} + \|\frac{\partial u}{\partial x}\|_{L^{2}(\Omega)}^{2}\right)^{\frac{1}{2}},$$
(3.9)

and semi-norm $|u|_{H^1}$ as follows:

$$|u|_{H^1} = \left(\left\| \frac{\partial u}{\partial x} \right\|_{L^2(\Omega)}^2 \right)^{\frac{1}{2}}, \tag{3.10}$$

accordingly, $H_0^1 = H_0^1(\Omega)$ is the Sobolev space $H^1(\Omega)$ that vanishes outside of a compact support on $\partial\Omega$ boundary of the domain. However, we are using $\|.\|_r$ for norm of sobolev space of $H^r(\Omega)$ which one can find a detailed definition in [12].

3.4 Weak Formulation

In this sequence, we introduce the classical weak formulation corresponding to equation (3.4). By multiplying this equation (3.4) by a test function $v \in V$, and using the Green's identity, the primal weak formulation of this problem is finding $u \in V$ such that

$$\left(\frac{\partial u}{\partial t}, v\right)_{\Omega} + a(u, v) = 0, \quad \forall v \in V,$$
(3.11)

where inner product of $L^2(\Omega)$ is denoted by (\cdot, \cdot) , and the bilinear form of $a(u, v) : V \times V \to \mathbb{R}$ is defined as follows:

$$a(u,v) := \left(\frac{1}{2}\sigma_{\epsilon}^{2}(u_{\epsilon}(x,t),t)\frac{\partial u_{\epsilon}}{\partial x},\frac{\partial v}{\partial x}\right)_{\Omega} + \left(\left(r + \frac{1}{2}\sigma_{\epsilon}^{2}(u_{\epsilon}(x,t),t)\right)\frac{\partial u_{\epsilon}}{\partial x},v\right)_{\Omega} + \left\langle\frac{\partial u_{\epsilon}}{\partial x},v\right\rangle_{\Gamma} + \left\langle u_{\epsilon},v\right\rangle_{\Gamma},$$
(3.12)

where Ω and Γ are the domain and the boundary of the problem respectively, and $\langle \cdot, \cdot \rangle$ is the duality pair that realized $L^2(\Gamma)$ in the sobolev space. It is worth mentioning that σ_{ϵ} implicitly depends on the solution of the problem. However, it should be noted that if the test function $v \in H_0^1(\Omega)$ has a compact support which vanishes on the boundary, the last two terms of (5.9) will disappear.

3.4.1 Some Properties of the Bilinear Form

In this part we will look closely at the bilinear form of equation (5.9) and study some of its basic properties that will be used for analyzing the method in the next sections. But, first we drop the ϵ subscript for the sake of simplicity as a conventional notation in derived results. We commence with this observation that the bilinear form (5.9) is bounded, so as a result, it is continuous as well. **Lemma 2**

Let's assume $X = H_1^0$ is the sobolev space of functions with compact support and $a : X \times X \longrightarrow \mathbb{C}$ is the bilinear form defined in (5.9), then we have

$$||a(u,v)|| \le C ||u||_1 ||v||_1 \quad \forall v \in H_1^0$$
(3.13)

where C is a constant depend on the volatilises.

Proof: To prove that (5.9) is bounded, one can observe that

$$|a(u,v)| = |(\frac{1}{2}\sigma^2 \frac{\partial u}{\partial x}, \frac{\partial v}{\partial x}) + ((r + \frac{1}{2}\sigma^2)\frac{\partial u}{\partial x}, v)|$$

using the triangle inequality and some simple calculations we will have

$$\leq |(\frac{1}{2}\sigma^2\frac{\partial u}{\partial x},\frac{\partial v}{\partial x})| + |((r+\frac{1}{2}\sigma^2)\frac{\partial u}{\partial x},v)|$$

now, using Cauchy-Schwarz inequality and assuming $C = \max\{(r + \frac{1}{2}\sigma_L^2), \frac{1}{2}\sigma_L^2\}$, and using sobolev embedding theorem [12] the desired result will be attained

$$\leq \frac{1}{2}\sigma^{2} \|u\|_{1} \|v\|_{1} + |(r + \frac{1}{2}\sigma^{2})| \|\frac{\partial u}{\partial x}\|_{L_{2}} \|v\|_{L_{2}} \leq C \|u\|_{1} \|v\|_{1}.$$
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.

The bilinear form (5.9) is not necessarily symmetric or positive definite depending on the value of volatilises and interest rate of the market. However, coercivity of this bilinear form can be shown as follows:

Theorem 7 (Coercivity)

Let $u \in H_0^1$, then the bilinear form of 5.9 satisfies the following inequality:

$$a(u,u) \ge C_1 \|u\|_1^2 - C_2 \|u\|^2, \quad \forall u \in H_0^1, \quad C_1 \in \mathbb{R}^+, C_2 \in \mathbb{R}$$
 (3.14)

where C_1 and C_2 are constants.

Proof: For any $u \in H_0^1$, since $||u||_{L_2}$ is bounded, we can add this term to the bilinear form as follows:

$$a(u, u) + C_2 \|u\|_{L_2}^2$$

 $= \left(\frac{1}{2}\sigma^2 \frac{\partial u}{\partial x}, \frac{\partial u}{\partial x}\right) + \left((r + \frac{1}{2}\sigma^2) \frac{\partial u}{\partial x}, u\right) + C_2(u, u)$

$$= \left(\frac{1}{2}\sigma^2 \frac{\partial u}{\partial x}, \frac{\partial u}{\partial x}\right) + \left(C_2 - \frac{1}{2}\left(\frac{\partial (r+\sigma^2)}{\partial x}\right)u, u\right)$$

 $\geq C_1 \|u\|_1^2 \quad \text{if} \quad C_2 > \sup \frac{1}{2}(r + \frac{1}{2}\sigma^2)$ where $C_1 = \min\{\frac{1}{2}\sigma_H^2, C_2 - \frac{1}{2}(r + \frac{1}{2}\sigma_H^2)\}$

The inequality (3.14) is a Gårding type inequality that provides a lower bound for the elliptic bilinear form. Having the continuity and coercivity of the bilinear form (5.9), the existence and uniqueness of the solution of the variational form (3.11) can be shown [27] for any function

belonging to Sobolev space $H_0^1(\Omega)$. Now, by proposition (7), obtaining result for the bilinear form of (5.9), we can investigate the stability of solution in the L_2 -norm in chapter (3.5). At the end of this section we briefly mention the adjoint operator of the corresponding bilinear form (5.9) that we will use to find approximately the free boundary as well as the error of the numerical method. Let's define an elliptic operator $L : H \to \mathbb{C}$ as follows:

$$(Lu, v) = -\left(\frac{1}{2}\sigma^2 \frac{\partial^2 u}{\partial x^2}, v\right) - \left(\left(r + \frac{1}{2}\sigma^2\right)\frac{\partial u}{\partial x}, v\right)$$
(3.15)

considering boundary condition of functions defined on the sobolev space H_0^1 , we can define an adjoint operator $L^* : \mathbb{C}^* \to H^*$ [86, 12, 26, 71] where

$$(u, L^*v) = -(\frac{1}{2}\sigma^2 u, v'') + ((r + \frac{1}{2}\sigma^2)u, v')$$
(3.16)

so, it is trivial that the operator L is not self-adjoint. Using the corresponding adjoint problem defined on adjoint operator (3.16) of elliptic problem based on bilinear form (5.9), we first find the error of finite element method for the corresponding elliptic problem in the next chapter. Then, we use this error of the finite element approximation to assess the error of the finite element method for the main problem (3.11) in L_2 Norm. Besides, in chapter (3.9) the Green function and this adjoint problem are used to explicitly estimate the free boundary which separates the high volatility region from low volatility region.

3.5 Analysis of Variational Form

In this chapter we analyze the variational form introduced in (3.11), then an approximation of the variational form via a finite element space is investigated in the following section. The free boundary problem introduced in system (3.4) can be considered as a convection diffusion problem. It is well-known that numerical algorithms can be unstable when the convection term is dominated-that is-coefficient of second order derivative is relatively small. First we show that the variational form introduced is bonded, meaning that the solution is stable through time and it is not going to blow up to infinity.

Theorem 8

Solution of u of variational form (3.11) satisfies the following stability estimate:

$$\|u(t)\| \le \|G(x)\| + C, \tag{3.17}$$

where C is a constant.

Proof: First let's choose v = u in the variational form of (3.11) and some trivial calculations and integration, and having proposition (7) in hand we have

$$(u_t, u) = -a(u, u),$$
 (3.18)

$$\frac{1}{2}\frac{d\|u\|^2}{dt} + C_1\|u\|_1^2 \le C_2\|u\|^2$$

and using Poincaré inequality for the first derivative we will have

$$\frac{1}{2}\frac{d\|u\|^2}{dt} \le C_1 \|u\|^2 + C_2 \|u\|^2, \tag{3.19}$$

now, integrating over time interval [0, t] yields

$$||u(t)|| \le ||G(x)|| + C_2 \int_0^t ||u|| ds,$$
 (3.20)

where the initial condition G(x) is defined in chapter (3.2). Now, by using Gronwall's lemma we will have

$$\|u(t)\| \le \|G(x)\| + C, \tag{3.21}$$

therefore, the desired result is attained.

Although the boundedness of the solution is obtained from proposition(8), we can make the bound even sharper for this problem.

proposition 3.5.1 Let's assume solution $u \in H_0^1$ satisfies the variational equation (3.11), it is stable by the mean of being bounded with the following bound

$$\|u(t)\| \le C_1 \|G(x)\| + C_2 \int_0^t \left\|\frac{\partial u}{\partial x}\right\| ds$$
(3.22)

where C_1 and C_2 are constants.

Proof: First let's again assume u = v in the variational form (3.11), so we have

$$(u_t, u) + a(u, u) = 0$$

In another word, we have the following variational equation:

$$(u_t, u) + (\frac{1}{2}\sigma^2 \frac{\partial u}{\partial x}, \frac{\partial u}{\partial x}) + ((r + \frac{1}{2}\sigma^2)\frac{\partial u}{\partial x}, u) = 0$$

$$\frac{1}{2}\frac{d}{dt}\|u\|^2 + \frac{1}{2}\sigma^2\left\|\frac{\partial u}{\partial x}\right\|^2 + |r + \frac{1}{2}\sigma^2|(\frac{\partial u}{\partial x}, u) = 0$$

Using cauchy-shwartz for the second and third terms, we have

$$\frac{d}{dt} \|u\|^2 + \sigma^2 \left\|\frac{\partial u}{\partial x}\right\|^2 \le 2|r + \frac{1}{2}\sigma^2| \left\|\frac{\partial u}{\partial x}\right\| \|u\|$$

Now using Poincaré inequality, we will have

$$\frac{d}{dt} \|u\| + \sigma^2 \left\| \frac{\partial u}{\partial x} \right\| \le 2|r + \frac{1}{2}\sigma^2| \left\| \frac{\partial u}{\partial x} \right\|$$

If we multiply both sides of the above equation by $e^{\sigma^2 t}$,

$$\frac{d}{dt}(e^{\sigma^2 t} \|u\|) + \sigma^2 e^{\sigma^2 t} \left\|\frac{\partial u}{\partial x}\right\| \le 2|r + \frac{1}{2}\sigma^2 |e^{\sigma^2 t} \left\|\frac{\partial u}{\partial x}\right\|$$

the left hand side of the above equation can be written as a complete differential

$$\frac{d}{dt}(e^{\sigma^2 t} \|u\|) \le 2|r + \frac{1}{2}\sigma^2|e^{\sigma^2 t} \left\|\frac{\partial u}{\partial x}\right\|$$
(3.23)

By integration from both sides, the left hand side will have the following form:

$$\int_0^t \frac{d}{dt} e^{\sigma^2 t} \|u\| = \|u(t)\| e^{\sigma^2 t} - \|u(0)\|$$

So, by substituting the above integration in the inequality of (3.23), and some calculations

$$\|u(t)\| \le e^{-\sigma^2 t} \|G(x)\| + 2|r + \frac{1}{2}\sigma(x)^2| \int_0^t \left\|\frac{\partial u}{\partial x}\right\| ds$$
(3.24)

now, assuming $C_1 := \sup\{e^{-\sigma(x)^2 t} | t \in [0, T], x \in \Omega = \Omega_H \cup \Omega_L\}$ and $C_2 := \sup\{|r + \frac{1}{2}\sigma(x)^2| x \in \Omega = \Omega_H \cup \Omega_L\}$ the bound will derive, which shows that the solution is stable with the above upper bound (3.24).

In this section, some stability properties of the variational form defined in (3.11) have been obtained. We showed that this form is well-defined and the solution of this variational form has an appropriate behavior for functions in the proper sobolev space $H_0^1(\Omega)$. Now, it is time to introduce the finite dimension approximation of this variational equation and study the accuracy and efficiency of the method.

3.6 Numerical Treatment with Finite Elements

In this section, we derive the primal formulation of credit rating migration problem from the variation form (3.11) using the standard Galerkin finite element method. Let U_h be the finite element subspace of Sobolev space $H^1(\Omega)$ generated by piecewise polynomials of degree $\leq r$, and V_h is the finite dimension subspace of test space V where boundary terms vanish on $\partial \Gamma$. In this investigation we use continuous Galerkin method, that is, both finite subspace of trail space H_0^1 and subspace of test space V overlaps meaning $V_h = U_h$. We define a partition $\mathcal{T}_h = \{T\}$ of sub-intervals such that $\Omega = \bigcup_{T \in T_h} T$, but not necessarily uniform of truncated spatial domain of $\Omega = [x_{min}, x_{max}]$ such that $x_{min} \leq x_1 \leq \cdots \leq x_{N_s} \leq x_{max}$, $h_i = x_{i+1} - x_i$ and $h = \max\{h_i, i \in 1, \cdots, N_s\}$. If we denote $u_h(t) = u(x_h, t)$, where $x_h \in \mathcal{T}_h$, the primal formulation of the credit rating migration is finding $u_h(t) \in V_h$ such that

$$\left(\frac{\partial u_h}{\partial t}, v_h\right)_{\Omega} + a_h(u_h, v_h) = 0, \quad \forall v_h \in V_h,$$
(3.25)

Where $a_h(u_h, v_h)$ is defined as approximate version of bilinear form as follows:

$$a_h(u_h, v_h) := \left(\frac{1}{2}\sigma^2(u_h(x, t), t)\frac{\partial u_h}{\partial x}, \frac{\partial v_h}{\partial x}\right)_{\Omega} + \left(\left(r + \frac{1}{2}\sigma^2(u_h(x, t), t)\right)\frac{\partial u_h}{\partial x}, v_h\right)_{\Omega}, \quad (3.26)$$

in fact, the equation (3.25) is semi-discrete and in order to fully approximate this equation numerically we discretize the time variable by the setting that $t_n = n\Delta t$ for $n \in \{1, \dots, N_t\}$, where $\Delta t = \frac{T}{N_t}$, and applying backward Euler

$$\left(\frac{u_h^n - u_h^{n-1}}{\Delta t}, v_h\right)_{\Omega} + a_h(u_h^n, v_h) = 0, \quad \forall v_h \in V_h,$$
(3.27)

where we used this notation convention $u_h^n := u(x_h, t_n)$. However, volatilises are computed implicitly with respect to the data from the previous steps. Expanding the solution u_h^n in a isoparametric form with the N_i for $i \in \{1, \dots, m\}$ of local piecewise continuous Lagrange shape functions of degree less than p like $u_h^n(\xi) = \sum_{i=1}^m u_i N_i(\xi)$, where ξ is the parent coordinate that can lead us to the following discrete system:

$$(\mathbf{K} + \Delta t \mathbf{M}) U^n = \mathbf{K} U^{n-1}, \qquad (3.28)$$

where vector $U^n = [u_1, \dots, u_{Ns}]^T$, N_s unknown of degrees of freedom on domain Ω_h , and **K** and **M** are stiffness and mass matrix corresponding with isoparametric form. It is not difficult to see that matrix on the left hand side of (3.28) is a positive definite and hence invertible [85].

3.7 Error Analysis of Finite Element Method

In this section, we analyze the approximate of the variational form in finite dimension space of the finite element space V_h . In order to show the error of approximation in L_2 , first we use the standard duality argument invented by Nitsche and Aubin [68, 5] to find the error analysis of the corresponding elliptic problem, then using this approximation, we investigate the accuracy of the finite element approximation for free boundary value problem (3.4). Let's recall the corresponding elliptic problem of variational form (3.11), this problem is seeking $u \in H_0^1$ which satisfies the following variation form:

$$a(u, v) = 0, \quad \forall v \in V = H_0^1,$$
 (3.29)

where bilinear form is defined in (5.9). Now, if we use the approximation via the finite element space V_h discussed in section (3.6), the discrete version of the problem (3.29) is finding $u_h \in V_h$ satisfying

$$a(u_h, v_h) = 0, \quad \forall v_h \in V_h, \tag{3.30}$$

now, let's assess the accuracy of this approximation in L_2 norm.

Theorem 9

Assume $u_h \in V_h$ is satisfying (3.30) to approximate the solution of the corresponding elliptic problem (3.29), then

$$\|u - u_h\|_{L_2} \le Ch^{r+1} \|u\|_{r+1} \tag{3.31}$$

and

$$\|u - u_h\|_1 \le Ch^r \|u\|_{r+1} \tag{3.32}$$

where C is a constant.

Proof: First, let's recall the adjoint bilinear form introduced in section (3.4.1)

$$a^*(u,u) = -(\frac{1}{2}\sigma^2 \frac{\partial u}{\partial x}, \frac{\partial v}{\partial x}) + (((r + \frac{1}{2}\sigma^2)u, \frac{\partial v}{\partial x}).$$

Assume if $\psi \in L^2(\Omega)$, we define $K(u) := \int_{\Omega} u\psi dx$, we can define the weak form of the dual problem pertain to (3.29) by seeking $\phi \in V$ such that

$$a^*(w,\phi) = K(w)$$
 (3.33)

Indeed, our adjoint problem is finding ϕ satisfying

$$\begin{cases} -\frac{1}{2}\sigma^{2}\frac{\partial^{2}\phi}{\partial x^{2}} + (r + \frac{1}{2}\sigma^{2})\frac{\partial\phi}{\partial x} = \psi, & \text{on} \quad \Omega, \\\\ \phi(x, 0) = G(x), & \\ \phi(x, t) = 0, & \text{on} \quad x \in \partial\Omega, \end{cases}$$
(3.34)

Now we can define the error of approximating K(u) by finite element space introduced in section (3.6) as follows:

$$K(u) - K(u_h) = \int_{\Omega} (u - u_h)\psi dx = -\left(\frac{1}{2}\sigma^2 \frac{\partial(u - u_h)}{\partial x}, \frac{\partial\phi}{\partial x}\right) + \left((r + \frac{1}{2}\sigma^2)(u - u_h), \frac{\partial\phi}{\partial x}\right), \quad (3.35)$$

using the definition of the adjoint operator, equation (3.35) equivalent to

$$K(u) - K(u_h) = -\left(\frac{1}{2}\sigma^2 \frac{\partial(u - u_h)}{\partial x}, \frac{\partial\phi}{\partial x}\right) - \left(\left(r + \frac{1}{2}\sigma^2\right) \frac{\partial(u - u_h)}{\partial x}, \phi\right),$$

besides, with the Galerkin orthogonality we know

$$a(u-u_h,\phi)=a(u-u_h,\phi-v),$$

so, by the continuity of the bilinear form one can show that

$$|K(u) - K(u_h)| \le C ||u - u_h||_1 \inf_{v \in V_h} ||\phi - v||_1,$$
(3.36)

by the regularity assumption on ϕ , adjoint problem (3.34), and finite element error results (see [12] for more details) we get,

$$\inf_{v \in V_h} \|\phi - v\|_1 \le Ch \|\phi\|_1 \le Ch \|\psi\|_{L^2},$$

thus, the desired error (3.36) is shown as

$$|K(u) - K(u_h)| \le Ch ||u - u_h||_1 ||\psi||_{L^2} \le ch^{r+1} ||u||_{r+1} ||\psi||_{L^2},$$
(3.37)

now, if we consider the special case of $\psi = u - u_h$, the error (3.36) will be

$$K(u) - K(u_h) = \int_{\Omega} (u - u_h)^2 dx = ||u - u_h||_{L^2}^2, \qquad (3.38)$$

substituting the above result (3.38) in inequality (3.37) yields

$$||u - u_h||_{L^2}^2 \le Ch||u - u_h||_1 ||u - u_h||_{L^2}$$

Therefore,

$$\|u - u_h\|_{L^2} \le Ch \|u - u_h\|_1 \le Ch^{r+1} \|u\|_{r+1}$$
(3.39)
In this proposition we proved the error bound for elliptic problem corresponding to the free boundary value problem using the Aubin-Nitsche duality argument. Now, we use this result to find the error of the finite element method to approximate the solution of 3.4. It is worth noticing that the technique used for this error is a common method that one can find in standard sources

[4, 85, 11].

Theorem 10

Assume that $u \in H_0^1$ is the solution of the free boundary value problem that satisfies the corresponding variational form (3.11), and $u_h \in V_h$ is the solution of the finite dimensional variational problem with finite element in (3.25), then

1. $\|u - u_h\|_{\infty} = O(h^{r+1})$ (3.40) 2. $\|u - u_h\|_{L_2} = O(h^r)$ (3.41)

Proof: Let's choose w_h as an elliptic projection of the exact solution u given by

$$\mathbf{a}(\mathbf{w}_h, \mathbf{v}) = \mathbf{a}(\mathbf{u}, \mathbf{v}), \quad \mathbf{v} \in \mathbf{V}_h, \quad 0 \le t \le T$$

In proposition (9) we studied the error of the finite element method approximating the elliptic operator as follows:

$$\|u(t) - w_h(t)\|_{L_2} \le Ch^{r+1} \|u(t)\|_{r+1}, \quad 0 \le t \le T$$
(3.42)

$$\|u(t) - w_h(t)\|_1 \le Ch^r \|u(t)\|_{r+1}, \quad 0 \le t \le T$$

Now, we differentiate with respect to time from both sides, and we know that time differentiation of u_h is elliptic projection of differentiation of u, so

$$\left\|\frac{\partial u(t)}{\partial t} - \frac{\partial w_h(t)}{\partial t}\right\|_{L_2} \le ch^{r+1} \left\|\frac{\partial u(t)}{\partial t}\right\|_{r+1}, \quad 0 \le t \le T$$
(3.43)

So, we have

$$\left(\frac{\partial w_h(t)}{\partial t}, v\right) + a(w_h, v) = \left(\frac{\partial w_h(t)}{\partial t}, v\right) + a(u, v) = \left(\frac{\partial (w_h - u)}{\partial t}, v\right), \quad v \in V_h, \quad 0 \le t \le T \quad (3.44)$$

If we assume $v_h = w_h - u_h$

$$\left(\frac{\partial v_h(t)}{\partial t}, v\right) + a(v_h, v) = \left(\frac{\partial (w_h - u)}{\partial t}, v\right), \quad v \in V_h, \quad 0 \le t \le T$$
(3.45)

If we use the differential representative of the first inner product in (3.45), and use Cauchy-Schwarz for the right hand side, we get

$$\|v_{h}\|_{L_{2}} \frac{d}{dt} \|v_{h}\|_{L_{2}} + a(v_{h}, v_{h}) = \left(\frac{\partial(w_{h} - u)}{\partial t}, v_{h}\right) \le \left\|\frac{\partial(w_{h} - u)}{\partial t}\right\|_{L_{2}} \|v_{h}\|_{L_{2}}$$
(3.46)

Therefore with simplification as well as the error bound of the projection (3.43) we will have

$$\frac{d}{dt} \|v_h\|_{L_2} \le \left\|\frac{\partial(w_h - u)}{\partial t}\right\|_{L_2} \le Ch^{r+1} \left\|\frac{\partial u(t)}{\partial t}\right\|_{r+1}$$
(3.47)

by integrating the above equation form 0 to T, we will get

$$\|\nu_{h}(t)\|_{L_{2}} \leq \|\nu_{h}(0)\|_{L_{2}} + \int_{0}^{T} (Ch^{r+1} \left\|\frac{\partial u(s)}{\partial s}\right\|_{r+1}) ds$$
(3.48)

if we assume u(0) is regular enough and we chose the initial data $u_h(0)$ such that $||u(0) - u_h(0)||_{L_2} = O(h^{r+1})$, we have

$$\|v_h(0)\|_{L_2} = \|w_h(0) - u_h(0)\|_{L_2} \le \|w_h(0) - u(0)\|_{L_2} + \|u(0) - u_h(0)\|_{L_2}$$
(3.49)

$$\leq Ch^{r+1} \|u(0)\|_{r+1} + \|u(0) - u_h(0)\|_{L_2} = O(h^{r+1})$$

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Now, by using the triangle inequality and both the results in H^1 and L_2 for the elliptic error estimate in (3.42) as well as the inequality of (3.49), we get the desired results.

The proposition (10) obtains an error bound for approximation of the finite element approximation.

3.8 Stability and Convergence of the Finite Element Method

In this section we investigate the stability and convergence of the discrete finite element method for solving the free boundary value problem (3.4). The variational form (3.11) has been discretized in the finite element space in spatial dimension (3.25) which eventuated in a set of ordinary differential equations. Then, we used backward Euler discretization in time to fully discretize the problem. First, let's study the stability of the method meaning that the solution is not going to blow up as time proceeds. In the following proposition we show that the discrete solution of u_h is bounded so it is stable numerically.

Theorem 11

Let u_h be the solution of the discrete system of (3.25), and volatility of the market satisfies in the following:

$$\sum_{n=1}^{n} \left[\sigma(u(t_n, x))^2 - \frac{\partial \sigma(u(t_n, x))^2}{\partial x} \right] \ge 0,$$
(3.50)

then, the finite element approximation is stable and we also have

$$\max_{1 \le n \le M} \|u^n\|_{L_2} \le C \|u^0\|_{L_2},\tag{3.51}$$

where *M* is the total number of time steps for Euler method, and *C* is a constant.

Proof: Assume $u_h \in V_h$ is the solution of fully discrete variational form of (3.25). We use an implicit Backward Euler finite difference to approximate the time derivative. so, we get

$$\left(\frac{u^{n} - u^{n-1}}{\Delta t}, v\right) + a_{h}(u^{n}, v, \sigma(u(t_{n-1}, x))) = 0, \quad v \in \forall V.$$
(3.52)

Note that in equation (3.52), bilinear form is unconventional and to some extent, imprecisely using third argument to emphasize dependency of volatility to the previous time step at each time step. By some elementary calculations we will have

$$(u^{n}, v) - (u^{n-1}, v) + \Delta t a_{h}(u^{n}, v, \sigma(u(t_{n-1}, x))) = 0,$$
(3.53)

$$(u^n, v) - (u^{n-1}, v) + \Delta t \left[\left(\frac{1}{2} \sigma(u(t_{n-1}, x))^2 \frac{\partial u^n}{\partial x}, \frac{\partial v}{\partial x} \right) + \left(\left(r + \frac{1}{2} \sigma(u(t_{n-1}, x))^2 \right) \frac{\partial u^n}{\partial x}, v \right) \right] = 0.$$

Let's write $u^n = \Delta t \frac{u^n - u^{n-1}}{2\Delta t} + \frac{u^n + u^{n-1}}{2}$, therefore the equation (3.53) can be rewritten as

$$\left(\frac{u^{n}-u^{n-1}}{\Delta t},\Delta t\frac{u^{n}-u^{n-1}}{2\Delta t}\right)+\left(\frac{u^{n}-u^{n-1}}{\Delta t},\frac{u^{n}+u^{n-1}}{2}\right)+a_{h}(u^{n},v,\sigma(u(t_{n-1},x)))=0,$$

utilizing the norm notation for inner products in Hilbet space, one gets

$$\frac{\Delta t}{2} \left\| \frac{u^n - u^{n-1}}{\Delta t} \right\|^2 + \frac{\|u^n\|^2 - \|u^{n-1}\|^2}{2\Delta t} + a_h(u^n, v, \sigma(u(t_{n-1}, x))) = 0.$$
(3.54)

Now, let's consider a special case of $v = u^n$ in equation (3.54), so the following equation will be attained

$$\frac{\Delta t}{2} \left\| \frac{u^n - u^{n-1}}{\Delta t} \right\|^2 + \frac{\|u^n\|^2 - \|u^{n-1}\|^2}{2\Delta t} + \frac{1}{2}\sigma(u(t_{n-1}, x))^2 |u^n|_1^2 - \frac{\partial}{\partial x}(r + \frac{1}{2}\sigma(u(t_{n-1}, x))^2) ||u^n||^2 = 0,$$
(3.55)

using Poincar \acute{e} -Friedrich inequality and considering the fact that a norm is always positive, the following inequality is valid

$$\frac{\|u^{n}\|^{2} - \|u^{n-1}\|^{2}}{2\Delta t} + \frac{1}{2}\sigma(u(t_{n-1}, x))^{2} \|u^{n}\|_{1}^{2} - \frac{\partial}{\partial x}(r + \frac{1}{2}\sigma(u(t_{n-1}, x))^{2})\|u^{n}\|^{2} \le 0,$$
(3.56)

so, sobolev embedding theorem for the second term of equation (3.56) will give us

$$\left[1 + \Delta t \left(\frac{1}{2}\sigma(u(t_{n-1}, x))^2 - \frac{\partial}{\partial x}(r + \frac{1}{2}\sigma(u(t_{n-1}, x))^2)\right)\right] \|u^n\|_{L_2}^2 \le \|u^{n-1}\|_{L_2}^2,$$
(3.57)

summing over all time steps through the time discretization, and assuming condition of (3.50), the proposition will be proved.

We showed in proposition (11) that the solution of discrete system (3.25) obtained from discretization of spatial variable by finite element and finite difference in time variable is bounded, that is, the discrete solution is numerically stable. In the next step, we study the simultaneous behavior of both linear Lagrange finite element and first order finite difference approximation of time derivative of variational problem (3.25) related to the credit risk migration and how algorithm is converging.

Theorem 12

Let u_h be the solution of the fully discrete system of (3.27) obtained by linear Lagrange finite element method on spatial variable and first order finite difference for time derivative, then we have

$$\max_{1 \le n \le M} \left\| u^n - u^n_h \right\|_{L_2} \le C(h^2 + \Delta t), \tag{3.58}$$

where *M* is the total number of time steps for Euler method, and *C* is a constant.

Proof: Let's start by assuming that w_h is the solution of the corresponding elliptic operator (3.30) such that

$$a(w_h, v_h) = a(u, v_h), \quad \forall v_h \in V_h,$$

we present the error $e_h^n := e(u(x_h, t_n))$ of approximating the solution of the variational form (3.25) as

$$e_h^n := u^n - u_h^n = \alpha^n + \beta^n,$$
 (3.59)
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where decomposition elements of α^n , and β^n are defined as follows:

$$\alpha^n = u^n - w_h^n, \tag{3.60}$$

$$\beta^n = w_h^n - u_h^n.$$

Using duality argument presented in section (3.7) in proposition(9), we get the following error bound for the linear finite element estimate of elliptic projection

$$\|\alpha^n\|_{L_2} \le Ch^2 |u^n|_2, \tag{3.61}$$

it is trivial that α also satisfies

$$a(\frac{\alpha^{n+1} - \alpha^n}{\Delta t}, v_h) = 0, \quad \forall v_h \in V_h$$
(3.62)

so by the inequality of (3.61), we get

$$\left\|\frac{\alpha^{n+1} - \alpha^n}{\Delta t}\right\|_{L_2} \le Ch^2 \left|\frac{u^{n+1} - u^n}{\Delta t}\right|_2,\tag{3.63}$$

besides, for n = 0 we can write,

$$(\beta^0, v_h) = (e_h^0, v_h) - (\alpha^0, v_h) = -(\alpha^0, v_h).$$
(3.64)

Now, let's consider a special case of $v_h = \beta^0$, by using Cauchy-Schwarz inequality we will have

$$\|\beta^0\|_{L_2} \le \|\alpha^0\|_{L_2} \le \frac{h^2}{p^2} |u^n|_2.$$
(3.65)

It is not difficult to see that β is satisfying the following:

$$\left(\frac{\beta^{n+1}-\beta^n}{\Delta t},v_h\right)+a(\alpha^{n+1},v_h)=\left(\frac{u^{n+1}-u^n}{\Delta t}-\frac{\partial u^n}{\partial t}-\frac{\alpha^{n+1}-\alpha^n}{\Delta t},v_h\right),$$
(3.66)

by the same procedure we prove the stability result in proposition (11), one can show that (see more details about duality argument in [5, 68])

$$\max_{1 \le n \le M} \|\beta^{n}\|_{L_{2}} \le \left[\|\beta^{0}\|_{L_{2}}^{2} + \sum_{n=1}^{N_{t}-1} \Delta t \|\vartheta^{n+1}\|_{L_{2}}^{2} \right]^{1/2},$$
(3.67)

where

$$\vartheta^{n+1} := \frac{u^{n+1} - u^n}{\Delta t} - \frac{\partial u^n}{\partial t} - \frac{\alpha^{n+1} - \alpha^n}{\Delta t}.$$
(3.68)

Since first term on the right hand side of (3.67) is estimated by the inequality of (3.65), so it remains to estimate the $\|\vartheta^{n+1}\|$, but we know from definition (3.68)

$$\left\|\vartheta^{n+1}\right\|_{L_2} \le \left\|\frac{u^{n+1} - u^n}{\Delta t} - \frac{\partial u^n}{\partial t}\right\|_{L_2} + \left\|\frac{\alpha^{m+1} - \alpha^n}{\Delta t}\right\|_{L_2} = I + II,\tag{3.69}$$

therefore, we need to assess the two components of (3.73). First term *I* on the right hand side of the recent equation can be rewritten as

$$\frac{u^{n+1}-u^n}{\Delta t} - \frac{\partial u^n}{\partial t} = -\frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} (t-t^n) \frac{\partial^2 u^n}{\partial t^2},$$
(3.70)

so we can show the following inequality for term I

$$I \leq \sqrt{\Delta t} \left(\int_{t^n}^{t^{n+1}} \left\| \frac{\partial^2 u^n}{\partial t^2} \right\|_{L_2} \right)^{1/2}.$$
(3.71)

1

inequality of (3.63) can be utilized for the second part *II* of inequality (3.69)

$$II \le Ch^2 \left| \frac{u^{n+1} - u^n}{\Delta t} \right|_2 = Ch^2 \left| \frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} \frac{\partial u^n}{\partial t} \right|_2 \le Ch^2 \sqrt{\Delta t} \left(\int_{t^n}^{t^{n+1}} \left| \frac{\partial u^n}{\partial t} \right|_2^2 dt \right)^{1/2}.$$
(3.72)

By substituting the bound for *I* and *II*, and using (3.67), and (3.65), we can find the bound for the β a component of error in (3.59)

$$\max_{1 \le n \le M} \left\| \beta^{m+1} \right\|_{L_2} \le C1(h^2 + \Delta t), \tag{3.73}$$

but, the error term defined in (3.59) is compound of α and β , thus it implies that

$$\max_{1 \le n \le M} \|u^n - u_h^n\|_{L_2} \le \max_{1 \le n \le M} \|\beta^n\|_{L_2} + \max_{1 \le n \le M} \|\alpha^n\|_{L_2}.$$
(3.74)

Thus, by considering two bounds of (3.73), and (3.61) we will have the

$$\max_{1 \le n \le M} \left\| u^n - u^n_h \right\|_{L_2} \le C(h^2 + \Delta t).$$
(3.75)

which finishes the proof. In the end, it is worth noticing that constant *C* is independent of *h*, and Δt and it varies from constants defined in inequality (3.72) and (3.63)

3.9 Dealing with Free Boundary

It is well-known that finding the free boundary where the volatility of firms switches between low and high credit grades is adding an extra complexity to the problem of rating migration. We must determine this boundary $S_f(t)$ where the solution u(x,t) at each time t reaches the value of $\gamma e^{-\delta t}$, where figure (3.1) illustrates figuratively this strategy. Besides finding this boundary value implicitly through solving the weak form and checking the occurrence of boundary value by ad-hoc method, we can estimate directly this free boundary value using green function and adjoint problem. To commence, we know that Green function $\varphi(s; x)$ for the system (3.4) satisfies in the following system of equations

$$\begin{cases} \varphi_t + L^* \varphi = \delta_s(x), & x \in \Omega, \\ \\ \varphi(s; x) = 0, & x \in \partial \Omega, \end{cases}$$
(3.76)

where L^* is the dual operator defined in (3.16), $\delta_s(x)$ is the delta function in x. It is easy to show that for each $s \in \Omega$ the solution of the weak form (3.11) satisfies the following:

$$u(s) = \int_{\Omega} \delta_s(x)u(x)dx = \int_{\Omega} \varphi_t u(x)dx + \int_{\Omega} \frac{1}{2}\sigma^2 \frac{\partial^2 \varphi}{x^2} u(x)dx + \int_{\Omega} (r + \frac{1}{2}\sigma^2) \frac{\partial \varphi}{x} u(x)dx, \quad (3.77)$$

now by setting $u(S_f) = \gamma e^{-\delta t}$ we will find the following nonlinear equation of

$$F_{\varphi(x,t)}(S_f) := \int_{\Omega} \varphi_t u(x) dx + \int_{\Omega} \frac{1}{2} \sigma^2 \frac{\partial^2 \varphi}{x^2} u(x) dx + \int_{\Omega} (r + \frac{1}{2} \sigma^2) \frac{\partial \varphi}{x} u(x) dx - \gamma e^{-\delta t} = 0.$$
(3.78)

Indeed, at each time t of time interval, boundary value $S_f(t)$ by estimating the unique root of the equation $F_{\varphi(x,t)}(s) = 0$ will be determined with standard an iterative method such as damped Newton method of the form of

$$x_{t_i,h}^{m+1} = x_{t_i,h}^m - \frac{F_{\varphi(x,t)}^h(x_{t_i,h}^m)}{F_{\varphi(x,t)}^{\prime h}(x_{t_i,h}^m)},$$
(3.79)

where $F_{\varphi(x,t)}^{h}$ is finite element discretization of the nonlinear system (3.78). Thus, this strategy can be used to explicitly approximate the free boundary of migration risk rate problem.

3.10 Numerical Results

In this section the efficiency and accuracy of the estimated methodology designed so far is examined by applying it on the example presented in [56]. We study the case when r = 0.5, $\delta = 0.005$, $\sigma_L = 0.3$, $\sigma_H = 0.2$, F = 1, $\gamma = 0.8$, T = 1. It is known [6, 56] that there is no analytical solution for the free boundary value problem (3.4). Thus, we used the numerical solution of the (3.4) via explicit finite difference proposed in [56] as a benchmark in order to compare the efficiency of our method. We used the $\Delta t = 1.0 \times 10^{-6}$ and $\Delta x = 1.0 \times 10^{-7}$ for the time steps and space steps respectively to attain this benchmark. We use finite element space V_h of degree r as investigated



Figure 3.1: Symbolically finding free boundary in time step t_n

in the previous sections. We use Lagrange basis for generating the finite element space and Guess quadrature rule for evaluating integrals. All the computations performed in MATLAB and linear system solved with backslash operator in MATLAB.

The errors that we compute here are $||E||_{L_2(\Omega)} = ||u - u_h||_{L_2(\Omega)}$, $||E||_{L_{\infty}(\Omega)} = ||u - u_h||_{L_{\infty}(\Omega)}$ and $||E||_{H_1(\Omega)} = ||u - u_h||_{H_1(\Omega)}$, where the exact solution is obtained as explained beforehand. We approximate the space of solution with the Lagrange finite element space of order *r* to study the accuracy of the high order finite element as well. Before proceeding further, let's mention again that we are estimating the time derivative with the first order finite difference method.

Table (3.1) showcases the error of estimating the solution with the finite element of order r = 1, 2, 3. Optimal order of convergence for approximating by a polynomial of order r for $||E||_{\infty}$ is r + 1, whereas the optimal order for $||E||_{L_2(\Omega)}$ is r (see proposition of (10)). However, we have not derived any theory about error in H1-norm, but numerical experiment shows that as we expect this

accumulative error of solution and first derivative of solution is higher than the two other norm, but order is consistent with L_2 -norm .that The order of convergence is consistent with the error estimate in (10)) and (12), and it is better than expected in high order estimation. For example when r = 3, we see that u_h converges with $O(h^{9/2})$ which is better than the optimal estimate. However, the last column of table (3.1) depicts that the method is rather expensive in terms of computational time especially as the order of the finite element method increases.

Table (3.2) illustrates the estimate solution for the linear finite element method verses the variate time steps. The optimal error convergence for error in L_2 norm is one (see proposition (12)). Besides, we try to experiment the time order for the H_1 norm with numerical simulations. Based on the result of the table (3.2), the estimated order $O(h^{1.091})$ is performing slightly better than the optimal order, whereas the estimate order for H_1 norm is less than one $O(h^{0.887})$. Finally, figure (3.2) illustrates the surface of the approximated solution with linear Lagrange finite element method.

Ne	r	$ E _{L_2}$	$ E _{H^{1}}$	$ E _{L_{inf}}$	Time(s)
1024	1	0.0167×10^{-3}	$0.0558. \times 10^{-3}$	0.0016×10^{-5}	0.8148
512	1	0.0335×10^{-3}	0.0995×10^{-3}	0.0014×10^{-5}	0.955
256	1	0.0674×10^{-3}	0.2392×10^{-3}	0.0280×10^{-5}	1.812
128	1	0.1352×10^{-3}	0.4253×10^{-3}	0.0993×10^{-5}	2.336
64	1	0.2703×10^{-3}	0.8326×10^{-3}	0.3858×10^{-5}	2.336
1024	2	0.0004×10^{-5}	0.0013×10^{-5}	0.0002×10^{-8}	0.814
512	2	0.0016×10^{-5}	0.0046×10^{-5}	0.0001×10^{-8}	0.955
256	2	0.0065×10^{-5}	0.0223×10^{-5}	0.0124×10^{-8}	1.812
128	2	0.0262×10^{-5}	0.0797×10^{-5}	0.0836×10^{-8}	2.336
64	2	0.1048×10^{-5}	0.3141×10^{-5}	0.6654×10^{-8}	2.336
1024	3	0.0001×10^{-9}	$0.0002. \times 10^{-8}$	0.0000×10^{-12}	0.814
512	3	0.0012×10^{-9}	0.0014×10^{-8}	0.0000×10^{-12}	0.955
256	3	0.0107×10^{-9}	0.0138×10^{-8}	0.0018×10^{-12}	1.812
128	3	0.0976×10^{-9}	0.0983×10^{-8}	0.0348×10^{-12}	2.336
64	3	0.8893×10^{-9}	0.7694×10^{-8}	0.7780×10^{-12}	2.336457

Table 3.1: Convergence Analysis of Finite Element Method, N_e is the number of elements, r represent the order of Lagrange shape functions

Table 3.2: Convergence analysis of time step with finite element method, N_t is number of time steps

N _t	$ E _{L_2}$	$ E _{H^1}$	Time(s)
1024	0.0035×10^{-5}	0.0146×10^{-3}	0.814
512	0.0130×10^{-5}	0.0293×10^{-3}	0.955
256	0.0484×10^{-5}	0.0694×10^{-3}	1.812
128	0.1807×10^{-5}	0.2017×10^{-3}	2.336
64	0.6750×10^{-5}	0.2343×10^{-3}	2.336



Figure 3.2: Approximated solution with linear finite element method

CHAPTER IV

THE DPG METHODOLOGY FOR QUANTITATIVE FINANCE

4.1 Option Pricing

In this chapter we utilize the DPG method introduced in section 1.3 to numerically solve the option pricing problem. In the sequence, DPG is exploited for vanilla options, American option, based on Black-Scholes model.

4.1.1 Black-Scholes Model

In this part, we use the DPG method for the popular Black-Scholes Model which simply provides a closed-form solution to all European-type Derivatives (vanilla option). It is worth mentioning that even though assumptions of this model are not worldwide valid, there are still a large group of people on the market that will use the Black-Scholes model plus a premium [40]. Besides, this model can be used as a test model to assess the efficiency of the method. Let's recall the Black-Scholes model briefly. This model assumes that the price of a risky asset, S_t , is evolving as a solution of the stochastic differential equation as follows

$$dS_t = rS_t dt + \sigma_t S_t dW_t, \tag{4.1}$$

in which W_t is the Wiener process on a appropriate probability space $(\Omega, \mathcal{A}, \mathbb{P}, \mathcal{F}_t)$, *r* is a risk free interest rate, and σ_t is volatility of the return on the underlying security. It is worth noticing that the SDE (4.1) is called geometric Brownian motion as well. Let's consider a European style

call option on an underlying asset S_t , where this spot price S_t satisfies in the geometric Brownian motion like (4.1) and with the payoff of max{ $S_T - K, 0$ } = ($S_T - K$)₊ at the date of expiration T for the striking price K. We are interested in the fair price of this option now denoted $U(S_0, 0)$, if we denote the value of the option by $U(S_t, t)$. The Black-Scholes formula express value of the option as

$$U(S_t, t) = \mathbb{E}^{Q}(e^{-\int t^T r_t dt} (S_T - K)_+ |\mathcal{F}_t),$$
(4.2)

It can be shown [1, 40] that option price of $U(S_t, t)$ satisfies in the followings deterministic partial differential equation.

$$\frac{\partial U}{\partial t} + \frac{\sigma^2}{2} S_t^2 \frac{\partial U^2}{\partial S^2} + rS \frac{\partial U}{\partial S} - rU(S, t) = 0$$
(4.3)

with the following boundary condition

$$U(0,t) = 0, \quad \forall t \in [0,T]$$

(4.4)

$$\lim_{S_t \to \infty} U(S_t, t) = S_t - e^{-r(T-t)} \quad \forall t \in [0, T]$$

It is well-known [78, 40, 1], having the upper tail of standard normal distribution

$$N(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-\frac{z^2}{2}} dz$$
(4.5)

and

$$d_{1} = \frac{\log(S_{0}/K) + (r + \frac{\sigma^{2}}{2}T)}{\sigma\sqrt{T}}, \qquad d_{2} = d_{1} - \sigma\sqrt{T}$$
(4.6)

the solution of equation (4.3) for a European call option can be expressed as

$$U(S_t, t) = S_t N(d_1) - K e^{-r(T-t)} N(d_2)$$
(4.7)

The closed-form analytical solution (4.7) for the European call option is used as a benchmark to study accuracy and efficiency of the DPG method. Switching log-prices $x = \log(\frac{S_t}{S_0})$, and changing

variable $\tau = T - t$, the partial differential equation (4.3), and the boundary conditions (4.3) can transfer to the following initial value constant coefficient partial differential equation

$$\begin{aligned} \frac{\partial U}{\partial \tau} &- \mathcal{L}_{BS} U = 0, \\ U(x, 0) &= \max(x - K, 0), \\ U(0, \tau) &= 0, \end{aligned}$$
(4.8)

where operator $\mathcal{L}_B S$ is defined as follows

$$\mathcal{L}_{BS} = -\frac{\sigma^2}{2} \frac{\partial U^2}{\partial x^2} - \left(r + \frac{\sigma^2}{2}\right) \frac{\partial U}{\partial x} + rU(x,t) = 0, \tag{4.9}$$

Noting that equation (4.8) can be used for pricing of derivatives whose payoff depends on the price of the underlying asset at the maturity date, and more complicated options whose prices are path-dependent such as American options and Asian options will use different approaches that we present them in coming sections. we use finite-difference θ -method to discretize the time derivative of the problem (4.8) with the followings form

$$\frac{u^{n+1} - u^n}{\Delta \tau} - (\theta \mathcal{L}_{BS} u^{n+1} + (1 - \theta) \mathcal{L}_{BS} u^{n+1}) = 0, \qquad (4.10)$$

for $n = 0, 1, 2, N_{\tau} - 1$, with the time step $\Delta \tau = T/N_{\tau}$, and implicitness factor $\theta \in [0, 1]$. so, different values for θ can lead us to different well-known time-stepping schemes such Backward Euler method ($\theta = 1.0$), Crank-Nicolson method ($\theta = 0.5$), and forward Euler method ($\theta = 0.0$). The Numerical efficiency of the finite difference method is well-known in the literature. we proceed with introducing the DPG methodology for spatial discretization. Varieties of the variational formulation can be developed for the semi-discrete model problem (4.10) with different properties. In this investigation, we concentrate on two formulations including the classical (primal) formulation and the ultraweak formulation.

4.1.2 Primal formulation for Vanilla options

In this subsection, we propose the standard classical variational formulation for the DPG method which is called the DPG primal formulation. Testing semi-discrete problem (4.10) with a proper test function v, integrating over the domain and using Green identity, we will have

$$(u^{n+1}, v) + \Delta \tau \theta \left[-\left(\frac{\sigma^2}{2} \frac{\partial}{\partial x} u^{n+1}, \frac{\partial}{\partial x} v\right)_{\Omega_h} + \left(\left(r + \frac{\sigma^2}{2}\right) \frac{\partial}{\partial x} u^{n+1}, v\right)_{\Omega_h} - \left(ru^{n+1}, v\right)_{\Omega_h} + \left(\frac{\partial}{\partial x} u^{n+1}, v\right)_{\partial \Omega_h} \right] + (u^n, v) + \Delta \tau (1 - \theta) \left[-\left(\frac{\sigma^2}{2} \frac{\partial}{\partial x} u^n, v\right)_{\Omega_h} + \left(\left(r + \frac{\sigma^2}{2}\right) \frac{\partial}{\partial x} u^n, v\right)_{\Omega_h} - \left(ru^n, v\right)_{\Omega_h} + \left(\frac{\partial}{\partial x} u^{n+1}, v\right)_{\partial \Omega_h} \right] = 0,$$

$$(4.11)$$

where (\cdot, \cdot) are standard inner product in the Hilbert space L_2 and $\langle \cdot, \cdot \rangle$ is the duality pair in the $L^2(\partial \Omega)$. Trial space is tested with a broader discontinuous (broken) space in the DPG methodology, so as a result we don't assume that test functions disappear on the Dirichlet boundary conditions. However, the term $\frac{\partial u}{\partial x}$ will be recognized as the flux variable \hat{q}_n which is a new unknown on the mesh skeleton. Thus, Defining a new group variable $\mathbf{u} = (u, \hat{q}) \in H_1(\Omega) \times H^{-1/2}(\partial \Omega)$, the broken primal formulation for Black-Scholes (4.8) reads

$$\begin{cases} b_{\text{primal}}(\mathbf{u}, v) = l(v), \\ \mathbf{u}(x, 0) = \max(x - K, 0), \\ \mathbf{u}(0, \tau) = 0. \end{cases}$$
(4.12)

where bilinear form $b_{\text{primal}}(\cdot, \cdot)$ and linear operator $l(\cdot)$ are defining as follows

$$b_{\text{primal}}(\mathbf{u}, v) = (u^{n+1}, v) + \Delta \tau \theta \Big[(-\frac{\sigma^2}{2} \frac{\partial}{\partial x} u^{n+1}, \frac{\partial}{\partial x} v)_{\Omega_h} + ((r + \frac{\sigma^2}{2}) \frac{\partial}{\partial x} u^{n+1}, v)_{\Omega_h} \\ -(u^{n+1}, v)_{\Omega_h} + \langle \hat{q}^{n+1}, v \rangle_{\partial \Omega_h} \Big], \qquad n = 1, \cdots, N_t,$$

$$l(v) = (u^n, v) + \Delta \tau (1 - \theta) \Big[(\frac{\sigma^2}{2} \frac{\partial}{\partial x} u^n, \frac{\partial}{\partial x} v)_{\Omega_h} + ((r + \frac{\sigma^2}{2}) \frac{\partial}{\partial x} u^n, v)_{\Omega_h} \\ -(u^n, v)_{\Omega_h} - \langle \hat{q}^n, v \rangle_{\partial \Omega_h} \Big], \qquad n = 1, \cdots, N_t,$$

$$\mathbf{u}_0 = \max(x - K, 0), \quad \forall x \in \Omega_h$$

$$\mathbf{u}_i(x = 0) = 0, \quad \forall i = 1, \cdots, N_t$$

$$(4.13)$$

It is worth mentioning again that here element-wise operations are denoted by subscribing h. The primal formulation (4.13) includes new flux unknown on the mesh skeleton, where we use a larger test space (enriched test space) to evaluate to repay these new variables.

4.1.3 Ultraweak Formulation for Vanilla options

In this section, we will derive the ultraweak formulation. the first step for finding ultraweak formulation is to transform the Black-Scholes problem (4.8) into a first-order system by defining a new variable $\vartheta(x, t) = \frac{\partial U}{\partial x}(x, t), \quad \forall (x, t) \in \Omega \times [0, T]$

$$\begin{cases} \frac{\partial U}{\partial \tau} - \frac{\sigma^2}{2} \frac{\partial \vartheta}{\partial x} - (r + \frac{\sigma^2}{2}) \vartheta + r U(x, t) = 0, \\ \vartheta - \frac{\partial U}{\partial x} = 0 \\ U(x, 0) = \max(x - K, 0), \\ U(0, \tau) = 0, \end{cases}$$
(4.14)

By defining a new group variable $\mathbf{u} = (u, \vartheta)$, testing the equation (4.14) with the test variables $\mathbf{v} = (v, \omega)$, and integrating and using Green's identity, we will have

$$(u^{n+1}, v) + \Delta \tau \theta \left[(\vartheta^{n+1}, \frac{\sigma^2}{2} \frac{\partial}{\partial x} v)_{\Omega_h} + (\vartheta^{n+1}, (r + \frac{\sigma^2}{2}) v)_{\Omega_h} - (u^{n+1}, v)_{\Omega_h} + -(u^{n+1}, \frac{\partial}{\partial x} \omega) - (\vartheta^{n+1}, \omega) + \left\langle \frac{\partial}{\partial x} u^{n+1}, v \right\rangle_{\partial \Omega_h} \left\langle \frac{\partial}{\partial x} \vartheta^{n+1}, v \right\rangle_{\partial \Omega_h} \right] + (u^n, v) + \Delta \tau \theta \left[(\vartheta^n, \frac{\sigma^2}{2} \frac{\partial}{\partial x} v)_{\Omega_h} + (\vartheta^n, (r + \frac{\sigma^2}{2}) v)_{\Omega_h} - (u^n, v)_{\Omega_h} + -(u^n, \frac{\partial}{\partial x} \omega) - (\vartheta^n, \omega) + \left\langle \frac{\partial}{\partial x} u^n, v \right\rangle_{\partial \Omega_h} + \left\langle \frac{\partial}{\partial x} \vartheta^n, v \right\rangle_{\partial \Omega_h} \right] = 0,$$

$$(4.15)$$

In order to use the DPG methodology, we use a discontinuous test space where this space is elementwise conforming. Besides, in ultraweak formulation there is no derivative of the trial variable in this weak formulation and these trial variable are defined in $L_2(\Omega)$, therefore, the boundary values of the field variables are meaningless on the skeleton. Thus, we introduce two trace variables $\hat{u}_{n+1} \in H^{1/2}(\Omega_h)$, and $\hat{\vartheta}^{n+1} \in H^{1/2}(\Omega_h)$ that are unknown on the skeleton. If we define the group variables $\mathbf{u} = (u, \vartheta)$, $\hat{\mathbf{u}} = (\hat{u}, \hat{\vartheta})$, and $\mathbf{v} = (v, \omega)$, the broken ultraweak formulation corresponding to the Black-Scholes model will be finding $\mathbf{u} = (u, \vartheta) \in L_2(\Omega) \times L_2(\Omega)$, and $\hat{\mathbf{u}} = (\hat{u}, \hat{\vartheta}) \in H^{1/2}(\Omega_h) \times H^{1/2}(\Omega_h)$ such that

$$b_{\text{ultraweak}}((\mathbf{u}, \hat{\mathbf{u}}), \mathbf{v}) = l(\mathbf{v})$$

($\mathbf{u}, \hat{\mathbf{u}}$)($x, 0$) = max($x - K, 0$), (4.16)
($\mathbf{u}, \hat{\mathbf{u}}$)($0, \tau$) = 0,

where

$$\begin{split} b_{\text{ultraweak}}((\mathbf{u}, \hat{\mathbf{u}}), \mathbf{v}) &= b_{\text{ultraweak}}(((u, \vartheta), (\hat{u}, \hat{\vartheta})), (v, \omega)) \\ &= (u^{n+1}, v) + \Delta \tau \theta \bigg[(\vartheta^{n+1}, \frac{\sigma^2}{2} \frac{\partial}{\partial x} v)_{\Omega_h} + (\vartheta^{n+1}, (r + \frac{\sigma^2}{2}) v)_{\Omega_h} - (u^{n+1}, v)_{\Omega_h} - (u^{n+1}, \frac{\partial}{\partial x} \omega) - (\vartheta^{n+1}, \omega) + \langle \hat{u}^{n+1}, v \rangle_{\partial \Omega_h} + \langle \hat{\vartheta}^{n+1}, v \rangle_{\partial \Omega_h} \bigg], \qquad n = 1, \cdots, N_t \end{split}$$

$$l(\mathbf{v}) = l(v,\omega) = (u^n, v) + \Delta \tau \theta \left[(\vartheta^n, \frac{\sigma^2}{2} \frac{\partial}{\partial x} v)_{\Omega_h} + (\vartheta^n, (r + \frac{\sigma^2}{2}) v)_{\Omega_h} - (u^n, v)_{\Omega_h} + (u^n, \frac{\partial}{\partial x} \omega) - (\vartheta^n, \omega) + \langle \hat{u}^n, v \rangle_{\partial \Omega_h} + \langle \hat{\vartheta}^n, v \rangle_{\partial \Omega_h} \right], \qquad n = 1, \cdots, N_t$$

$$(\mathbf{u}, \hat{\mathbf{u}})^0 = \max(x - K, 0),$$

 $(\mathbf{u}, \hat{\mathbf{u}})^i = 0, \qquad n = 1, \cdots, N_t$ (4.17)

It is well-known fact [19, 20], that the DPG method significantly depends on the choice of the test space inner product since it determines the norm and as a result the structure of test space in which the DPG method is optimal. As an illustration, if the errors in L_2 -norm are of interest, there is a tangible theory [21] that shows that the graph norm is a suitable choice for the test space in ultraweak formulation, and the standard energy norm induced form bilinear $\|\cdot\|_E = b_{\text{primal}}(v, v)$ is the candidate the primal formulation. we employ the following test norms for the formulations proposed above. In this paper, we propose the following graph norm (4.16), and (4.12)

Primal :
$$\|v\|_V^2 = \frac{1}{\Delta t} \|v\|^2 + \frac{1}{(\Delta t)^2} \|\frac{\sigma^2}{2} \frac{\partial}{\partial x} v\|^2$$
, (4.18)

Ultraweak :
$$\|\mathbf{v}\|_V^2 = \|(v,\omega)\|_V^2 = \frac{1}{(\Delta t)^2} \|c5\frac{\partial}{\partial x}v - c6v - \omega\|^2 + \frac{1}{\Delta t} \|c7v - \frac{\partial}{\partial x}\omega\|^2$$
,

Having the graph norm and energy norm defined above, and as a direct result of the inner product of the test space, we are ready to discretize the ultraweak form and construct the DPG system. In the classical Galerkin method, the convention is to choose the same discrete space for both trial and test spaces, so a squared linear system is expected. However, in the DPG method, discrete trial $U_h \subset U$ and test space $V_h \subset V$ have different dimensions. The practical DPG method with optimal test space benefits from enriched test space, meaning that dim $V_h \ge \dim U_h$. We assume that $\{u_j\}_{j=1}^N$, and $\{v_j\}_{j=1}^M$ are the bases of trial and test spaces respectively where $M \ge N$. In the DPG methodology, each trial space basis function u_i and corresponding optimal test function v_i^{opt} satisfy the following system

$$(v_i^{\text{opt}}, \delta v)_V = b(u_i, \delta v), \quad \forall \delta v \in V$$
 (4.19)

Now let's define $M \times M$ Gram matrix $G = (G_{ij})_{M \times M}$

$$G_{ij} = (v_i, v_j)_V$$

and $N \times M$ stiffness matrix $B = (B_{ij})_{N \times M}$

$$B_{ij} = b(u_i, v_j)$$

for primal formulation finding matrix B is straightforward from the bilinear form and test norm, however, calculating this matrix for ultraweak formulation can be confusing, where B having the following structure

$$B = \begin{bmatrix} B_{uv} & B_{\vartheta v} & B_{\hat{u}v} & B_{\hat{\vartheta}v} \\ B_{u\omega} & B_{\vartheta \omega} & B_{\hat{u}\omega} & B_{\hat{\vartheta}\omega} \end{bmatrix}_{N \times M}$$
(4.20)

and *l* the mass matrix l(v) = (f, r). We use high order Lagrange basis of different order to expand the trial space with order *P*, and enriched test space with order $p + \Delta p$ for $\Delta p = 1, 2, \cdots$. The global assembly will have the following form

$$B^{\text{n-op}}\mathbf{u}_h = B^T G^{-1} B \mathbf{u}_h = B^T G^{-1} l = l^{\text{n-op}}$$
(4.21)

where discrete operators B^{n-op} , and l^{n-op} are near optimal mass and stiffness matrix for DPG formula. It is worth noting that thanks to the broken structure of the test space, evaluating optimal test functions in Gram matrix and its inversion are localized and therefore the global assembly can be paralleled, which makes the DPG method a practical method to solve the option pricing problem.

4.1.4 Greeks

In this section, we provide numerical tools based on collocation meshfree methods to calculate the sensitivity of the option pricing under generalized fractional Brownian motion. The sensitivity of option prices with respect to underlying variables which are called "Greeks", is significantly important for market makers in the derivative markets. Traders by considering Greeks are able to achieve a certain risk by changing the quantities of these options in their portfolio. Besides, monitoring these sensitivities help the traders to hedge their portfolio by using other derivatives as a buffer to overcome significant market changes. these Greeks are using computed by partial differentiation of the price of a derivative concerning the desired underlying variable. in the following First Greeks that we study in this section is Delta which is sensitive to the option with respect to the asset price and is shown as follows

$$\Delta = \frac{\partial u(S,t)}{\partial S},\tag{4.22}$$

It is well-known that Delta for the call option is positive, whereas this sensitivity for the put option is negative. The second Greek that we study here is Gamma which is

$$\Gamma = \frac{\partial^2 u(S,t)}{\partial S^2},\tag{4.23}$$

this Greek shows the immediate change of Greek defined in (4.23), which is calculated by the second derivative of the price of the contract with respect to the asset price. In this sequence, we can define high order Greeks such as Speed which is the third derivative and Dspeed Greek that is the sensitivity of option with respect to the underlying speed define as follows

Speed =
$$\frac{\partial^3 u(S,t)}{\partial S^3}$$
, Dspeed Dspot = $\frac{\partial^4 u(S,t)}{\partial S^4}$, (4.24)

In addition to the sensitivity that measures the change in asset price, time decay is very essential for traders in the market. Time decay can be measured by the Theta which is defined as following

$$\Theta = \frac{\partial u(S,t)}{\partial t},\tag{4.25}$$

This Greek indicates the change of price of the option with respect to the time as the option advance to its expiration. There are other Greeks such as sensitivity with respect to volatility or interest rate that are less common that we ignore in this section.

4.1.5 Numerical Results

In this section, we provide numerical experiments to showcase the efficiency and accuracy of the DPG method in valuing vanilla options using both primal and ultraweak DPG methods. For this experiment, the risk-free rate r is set to be 0.05, the time to maturity T is one year, and the strike price K is 100. The computational domain is [-6, 6], and a variety of values for the volatility of the market σ . In this paper, we report the relative errors of L_2 , L_{∞} of the solution. we used the binomial method implemented in [39] as a benchmark and analytical solution to compare with the approximated solution obtained with the DPG method. The relative errors are defined as follows

$$\|E\|_{L_2}^2 = \|\frac{u - \tilde{u}}{u}\|_{L_2}^2 \qquad \|E\|_{\infty} = \|\frac{u - \tilde{u}}{u}\|_{L_{\infty}}$$
(4.26)

where \tilde{u} represents the estimated value attained from numerical method. Figure (4.1) depicts the surface of a call option with volatility $\sigma = 0.4$ for both primal and ultraweak DPG formulation.

In this part of experiment, we study the asymptotic convergence of relative errors of numerical method for uniform mesh refinement both in time and steps. In this regard Fig. (4.2) displays the space order of convergence of the primal DPG method for volatilises of $\sigma = 0.3$ and $\sigma = 0.015$. It is evident that convergence rate of the primal DPG scheme is super linear in space. the same investigation for the ultraweak DPG scheme (4.4) shows that although convergence rate in space is super-linear the errors in this scheme decay moderately gentle. we observe that for the space order in both ultraweak and primal scheme initially we see some inconsistency in linear decreasing of the error but once number of elements approaches to a certain point we witness the expected linear O(h) which can cause this overall super linear convergence



Figure 4.1: The option price surface for $\sigma = 0.4$, and r = 0.1 using the ultraweak and primal DPG formulations.

rate. However, Fig. (4.3), and Fig. 4.5 depicts this observation more precisely when for the same scenario the rate of convergence for the Primal DPG and the Ultraweak DPG method is linear in time due to the fact that the h = 0.01 is fixed for this experiment.



Figure 2: Global Error of DPG formulation for European option with parameters: r=0.05, $\sigma=0.15$, K=100



Figure 4.2: (Space Order)Accuracy properties of the primal DPG for European put options r=0.05, K=100, and different volatility

4.1.6 American options

In this section, we briefly review American option pricing under the simple model of Black-Scholes. Contrary to the European option, the holder of this contract has the right to exercise the option at any time before maturity. It is well-known that this slight difference brings the analysis of American options much more complicated. Indeed, this right turn problem of valuing American options into a stochastic optimization problem. The price of an American option under the risk-neutral pricing principle can be obtained as

$$U(x,t) = \sup_{t \le \tau \le T} \mathbb{E}[e^{-r(\tau-t)}h(x)]$$
(4.27)

where h(x) is the option payoff, and τ is a stopping time. This stopping time is the time that owner of the option exercises the contract, besides, this stopping time is a concept in the stochastic analysis as well. It is worth noting that due to the complexity of the American option problem, this problem does not have a



Figure 4.3: (Space Order)Accuracy properties of the primal DPG for European put options r=0.05,

K=100, and different volatility



Figure 4.4: (Space Order)Accuracy properties of the primal DPG for European put options r=0.05, K=100, and different volatility

closed-form solution. One way of formulating the American option thanks to the no-arbitrage principle is the free boundary value problem. Indeed, this free boundary happens when the option is deep-in-the-money,



Figure 4.5: (Space Order)Accuracy properties of the primal DPG for European put options r=0.05, K=100, and different volatility

and finding this boundary alongside pricing the American option brings extra difficulties to the problem. Here we briefly recall the different forms of presenting American options and the DPG formulation for the pricing the corresponding forms.

Considering the log-prices $x = \log(\frac{S_t}{S_0})$, changing tenor T - t to τ , the free boundary formulation of the American put option yields:

$$\begin{split} \frac{\partial U}{\partial \tau}(x,\tau) &- \frac{\sigma^2}{2} \frac{\partial U^2}{\partial x^2}(x,\tau) - \left(r + \frac{\sigma^2}{2}\right) \frac{\partial U}{\partial x}(x,\tau) + rU(x,\tau) \le 0, \quad \forall x > S_f, \\ U(x,\tau) &= K - e^x \quad \forall x \le S_f, \\ U(x,0) &= (K - e^x)^+, \\ \lim_{x \to \infty} U(x,\tau) &= 0, \\ \lim_{x \to S_f} U(x,\tau) &= K - e^{S_f}, \\ \lim_{x \to S_f} \frac{\partial U(x,\tau)}{\partial x} &= -1, \end{split}$$
(4.28)

in which, S_f is the free boundary of the American option pricing. There is another approach to deriving American option pricing called a linear complementarity problem (LCP). The advantage of this approach is that free boundary is not present in the formulation anymore. However, solving the LCP problem has its complexity. The complementarity problem of the American option can be written as

$$\left(\frac{\partial U}{\partial \tau}(x,\tau) - \frac{\sigma^2}{2}\frac{\partial U^2}{\partial x^2}(x,\tau) - (r + \frac{\sigma^2}{2})\frac{\partial U}{\partial x}(x,\tau) + rU(x,\tau)\right)(U(x,\tau) - h(x)) = 0,$$

$$\frac{\partial U}{\partial \tau}(x,\tau) - \frac{\sigma^2}{2}\frac{\partial U^2}{\partial x^2}(x,\tau) - (r + \frac{\sigma^2}{2})\frac{\partial U}{\partial x}(x,\tau) + rU(x,\tau) \ge 0,$$

$$U(x,\tau) - h(x) \ge 0,$$

$$U(x,0) = (K - e^x)^+.$$
(4.29)

The main approach here is to utilize the DPG formulation for the governing equations of the Equ. (4.29) and then consider the free boundary condition for them. This approach is examined before in [30] for using DPG formulation for Signorini type problem as a contact problem. However, Thomas Fuhrer et al. in [30] proposed the ultraweak formulation of the Signorini problem, here we derive both ultraweak and primal formulation of the DPG method for the problem of American option pricing as a special case of obstacle problem. So, if we multiply the second inequality condition with the smooth no-negative test functions $v \in V^0$ where test space is a broken convex cone and following the same process of defining trail and flux variable presented in the previous section, and after some integration by part we obtain

$$\frac{d}{d\tau}(\mathbf{u}, \mathbf{v}) + b^{\tau}(\mathbf{u}, \mathbf{v}) \ge 0, \tag{4.30}$$

where bilinear form for primal formulation defies as

$$b_{\text{primal}}^{\tau}(\mathbf{u}, v) = \left(-\frac{\sigma^2}{2}\frac{\partial}{\partial x}u, \frac{\partial}{\partial x}v\right)_{\Omega_+} + \left(\left(r + \frac{\sigma^2}{2}\right)\frac{\partial}{\partial x}u, v\right)_{\Omega_+} - (u, v)_{\Omega_+} + \langle \hat{q}, v \rangle_{\partial\Omega_+}, \tag{4.31}$$

with a set of trial and flux variables $\mathbf{u} = (u, \hat{q}) \in V(\Omega) \times V^{\frac{1}{2}}(\partial \Omega)$, test variable $\mathbf{v} = v \in V^{0}(\Omega)$. Moreover, considering trail variables $\mathbf{u} = (u, \vartheta) \in L_{2}(\Omega) \times L_{2}(\Omega)$, and flux variables $\hat{\mathbf{u}} = (\hat{u}, \hat{\vartheta}) \in H^{1/2}(\partial \Omega_{h}) \times H^{1/2}(\partial \Omega_{h})$ the bilinear form (4.30) for the ultraweak formulation reads

$$b_{\text{ultraweak}}^{\tau}((\mathbf{u}, \hat{\mathbf{u}}), \mathbf{v}) = b_{\text{ultraweak}}^{\tau}(((u, \vartheta), (\hat{u}, \hat{\vartheta})), (v, \omega))$$
$$= (\vartheta, \frac{\sigma^2}{2} \frac{\partial}{\partial x} v)_{\Omega_+} + (\vartheta, (r + \frac{\sigma^2}{2}) v)_{\Omega_+} - (u, v)_{\Omega_+} - (u, \frac{\partial}{\partial x} \omega)_{\Omega_+}$$
$$-(\vartheta, \omega)_{\Omega_+} + \langle \hat{u}, v \rangle_{\partial\Omega_+} + \langle \hat{\vartheta}, v \rangle_{\partial\Omega_+}.$$
(4.32)

It is well-known that the two variational inequality proposed above are the parabolic variational inequalities of the first kind that admit a unique solution. It is evident that test space V^0 can be written as $V^0 = h(x) + V^0_+$, where the space of V^0_+ is the cone of positive functions in V. Having well-posed variational inequality of (4.30), we can approximate the problem in a finite dimensional space. Thus, similar to the estimating vanilla options, we introduce the time partition of $0 \le \cdots \le T$ of the time interval [0,T], and discrete trial $U_h \subset U$, and enriched test space $V_h \subset V$ (dim $V_h \ge \dim U_h$) and the corresponding basis that $\{u_j\}_{j=1}^N$, and $\{v_j\}_{j=1}^M$ for the aforementioned spaces. we use the backward finite difference Euler method to approximate the time derivative, and as a result, the discrete DPG for variational inequalities arising from American option pricing problem yields

$$(u^{n+1} - u^n, \mathbf{v}) + \Delta \tau b_n^\tau (u^n, \mathbf{v}) \ge 0, \quad \forall \mathbf{v} \in V_h.$$

$$(4.33)$$

However, writing the θ -method for the second term of the discrete variational inequality (4.33) will be performed very similarly to what is proposed for vanilla options. Let *B* and *G* be the Gram matrices defined by

$$B_{ij} = b^{\tau}(u_i, \mathbf{v}_j), \quad G_{ij} = (\mathbf{v}_i, \mathbf{v}_j)_{\nu}, \quad l_i = (u_i, \nu)$$
 (4.34)

where $(\cdot, \cdot)_{\nu}$ inner product of test space with the energy norm for primal DPG and graph norm for ultraweak form introduced in (4.18). So, the discrete variational inequality (4.33) is equivalent to

$$B^{T}G^{-1}l(u^{n+1} - u^{n}) + \Delta\tau B^{T}G^{-1}Bu^{n} \ge 0,$$

$$u^{n} \ge h(x),$$

$$(4.35)$$

$$(u^{n} - h(x))(B^{T}G^{-1}l(u^{n+1} - u^{n}) + \Delta\tau B^{T}G^{-1}Bu^{n}) = 0.$$

for $n = 1, \dots, N_{\tau}$ by setting near the optimal discrete operations of $B^{n-op} = B^T G^{-1} B$, $l^{n-op} = B^T G^{-1} l$ discrete LCP (4.35) will attain the following form

$$\begin{cases} l^{n-op}(u^{n+1} - u^n) + \Delta \tau B^{n-op} u^n \ge 0, \\ u^n - h(x) \ge 0, \qquad \forall n = 1, \cdots, N_{\tau}, \\ (u^n - h(x)) (l^{n-op}(u^{n+1} - u^n) + \Delta \tau B^{n-op} u^n) = 0. \end{cases}$$
(4.36)

There are different approaches to solve the discrete variational inequality (4.36) including fix-point approach, penalization method, iterative method to just name few [16].

4.1.7 Numerical Experiments

In this set of numerical experiments, we study the problem of valuing the American option with the ultraweak and primal DPG method. we aim for verifying that DPG is a reliable and stable method for solving this free boundary value problem. Error convergence analysis conducted with the relative L_2 , and L_{∞} error of the solution similar to definitions (4.26). Fig 4.6 illustrates the order of convergence of both formulation for valuing American option for interest rate r = 0.05, K = 100, and $\sigma = 0.15$ in space order for first order and second order DPG. This experiment shows that asymptotic convergence of L_2 error is super linear, but it doesn't reach the $o(h^2)$ for the second-order DPG. One possible reason could be the impact of free boundary that deteriorate the rate of convergence for the method. However, the error is relatively small, and table (4.1) reinforces this trend as well for relative sup-error for both primal and ultraweak formulation, where ultraweak formulation has a tiny better performance in the majority of cases. To study the stability and convergence in the time-stepping scheme, we prepared Fig. (4.7). we used a fixed mesh of 64 elements

and decrease the time step $\Delta \tau$. The convergence analysis shows that both primal and ultraweak formulation benefit from the rate of convergence of $O(\Delta \tau)$ as we expected and as a result the backward Euler method is unconditionally stable. However, the rate of convergence for time-stepping captures for initial time steps, and spacial discretization dictates its impact afterwards for both DPG forms.



Figure 4.6: (space order)Accuracy properties of primal (left) and ultraweak (right) DPG for American put options r=0.05, K=100, and $\sigma = 0.15$

It is a well-known fact that the price of an American option is bigger than European option due to the having right of the owner of the American option for exercising anytime before maturity, this is can be seen in Fig. (4.8) for the payoff of an American option. The proposed methods can capture this behavior accurately for different volatility of the market for both primal and ultraweak formulation Fig. (4.9).

Besides pricing accurately the American option, finding the optimal exercise boundary for an American option is very important. The DPG method proposed in this section can find this free boundary implicitly thanks to the projection-based method just by checking the price with the payoff at each moment or automatically first active points at each time step in the primal-dual active set strategy. Fig. (4.10) depicts

Δau	h	value		$\ E\ _{\infty}$
		Primal	Ultraweak	Primal Ultraweak
0.01	0.46	14.	15.	0.0159930 0.00963025
10	0.23	14.	15.	0.00379765 0.00050253
10	0.11	14.	15.	0.00074574 0.00133183
10	0.05	14.	15.	0.00034449 0.00027304
10	0.03	14.	15.	5.83E-05 6.21E-05
10	0.02	14.	15.	4.12E-05 4.48E-05
10	0.01	14.	15.	1.77E-05 1.75E-05

Table 4.1: Value of American Option r = 0.05, σ = 0.15, k = 100



Figure 4.7: (Time order) Accuracy properties of Ultreawek and primal DPG for American put options r=0.05, K=100, and $\sigma = 0.15$

finding this free boundary for the different interest rates of the market at each time. Thus this optimal exercise boundary partitions the domain of the problem into an "Exercise region" and "Do not Exercise"



Figure 4.8: American put premiums for r=0.05, K=100, and $\sigma = 0.5$



Figure 4.9: Value of American option for r=0.05, K=100, and different volatilises

region (4.10) where the owner of the option will exercise the option when the stock price is at the Exercise region.



Figure 4.10: Optimal Exercise boundary for an American put. Computed via the primal DPG method. b) the green part is for exercise and red for "Do not exercise"

CHAPTER V

THE DPG METHOD FOR STRUCTURAL MECHANICS

In this chapter, we propose a new Discontinuous Petrov-Galerkin method to numerically analyze a onedimensional Reissmer-Mindlin plate model which is a Timoshenko beam model. The governing equation arising from this problem can be reduced to a fourth-order partial differential equation, and the numerical method proposed to approximate its solution is automatically stable and lock-free. Numerical solutions illustrate the efficiency and convergence of the method especially when the thickness of the beam tends to zero.

5.1 Introduction

Problems from solid mechanics pertaining to structures such as beams, plates, and shells have been increasingly attracting scientists due to their myriad fields of application. The corresponding one-dimensional case of the Reissmer-Mindin plate is the Timoshenko model for beam bending. The importance of studying a one-dimensional model is that it can pave the way to design a reliable numerical algorithm for more complicated structures like shells. However, the thickness parameters in these models of solid mechanics can have an adverse effect on the efficiency of numerical models designed to tackle the aforementioned problems. These effects in engineering literature are known as shear and membrane locking.

There is a wide variety of numerical methods that have been devised on the Timoshenko beam problem. However, it is worth mentioning that Fatih Celiker et al.[14] used the discontinuous Galerkin method to analyze the Timoshenko beam. They studied the quality of the numerical method with respect to the thickness of the beams. Later, Niemi and his colleagues [67] used the Discontinuous Petrov-Galerkin method for beam theory and especially cantilever with tip load. However, the DPG method used in [67] is not the DPG method with optimal test space created by Demkowicz and Gopalakrishnan [21].

In this section, we propose a Discontinuous Petrov-Galerkin method (DPG) with optimal test space for modeling the Timoshenko beam problem. The Discontinuous Petrov-Galerkin developed by Demkowicz and Gopalakrishnan benefits from very interesting properties for the numerical approximation of scientific research. In this method, discrete stability is guaranteed by choosing an optimal test space such that the inf-sup condition is satisfied. DPG method for estimating solution space of fourth-order partial differential equation arising from Timoshenko beam theory is used and its computational results illustrate that the method is lock-free and stable. Investigating broadly the properties of the method, the results will be provided for different boundary conditions.

5.2 Model Problem and Ultraweak Formulation

According to the beam theory, the governing equations modeling a beam on a domain $\Omega = [0, T]$ with length *L* under a transverse load *q* are as follows:

$$\begin{cases} \frac{\partial}{\partial x} \left(EI_A \frac{\partial \theta_y}{\partial x} \right) + GA\kappa \left(\frac{\partial u}{\partial x} - \theta_y \right) = \rho I_A \frac{\partial^2 \theta_y}{\partial t^2}, \\ \frac{\partial}{\partial x} \left(GA\kappa \left(\frac{\partial u}{\partial x} - \theta_y \right) \right) = -q + \rho A \frac{\partial^2 u}{\partial t^2}. \end{cases}$$
(5.1)

in which u(x, t) is the transverse displacement and θ_y is the rotation angle of the normal to the mind surface of the beam. The elastic modulus and shear modulus are shown by *E* and *G* respectively, κ is the shear correction factor, ρ is the density, the cross section area is *A*, and *I_A* is the moment of inertia. In this work, we choose to work with the static Timoshenko equation where Euler-Bernouli theory is a special case of the beam theory. In fact, this model will be reduced to a forth order partial differential equation which has a second derivative as well.
Therefore, the steady state Timoshenko equation when $\frac{\partial u}{\partial t} = \frac{\partial \theta_y}{\partial t} = 0$, is as follows:

$$\frac{\partial}{\partial x} \left(E I_A \frac{\partial \theta_y}{\partial x} \right) + G A \kappa \left(\frac{\partial u}{\partial x} - \theta_y \right) = 0,$$

$$- \frac{\partial}{\partial x} \left(G A \kappa \left(\frac{\partial u}{\partial x} - \theta_y \right) \right) = q.$$
(5.2)

It is trivial to see that when we ignore the shear strain, i.e., $\theta_y - \frac{dv}{dx} = 0$, the Euler-Bernoulli equation is attained. The Euler-Bernoulli equation is given by:

$$EI_A \frac{d^4v}{dx^4} = q.$$

Besides, Dirichlet boundary conditions for the system (5.2) are

$$\begin{cases} D|_{\Gamma_D} = u_D, \\ \theta_y|_{\Gamma_D} = \theta_{y_0}, \end{cases}$$
(5.3)

and Neumann boundary conditions are given as

$$\begin{pmatrix} \hat{n} \cdot GA\kappa(\theta_y - \frac{dv}{dx}) \end{pmatrix}|_{\Gamma_N} = f_1,$$

$$\begin{pmatrix} \hat{n} \cdot EI_A \frac{d\theta_y}{dx} \end{pmatrix}|_{\Gamma_N} = f_2,$$

$$(5.4)$$

in which u_D , θ_{y_0} , f_1 , and f_2 are known functions. It is obvious that different combinations of the boundary conditions (5.3) and (5.4) can produce all the physically corresponding boundaries of the free end, supported end, and clamped end. In the next section, we derive the ultraweak formulation pertaining to (5.2) which is used for the DPG method.

5.3 Ultraweak Formulation of Timoshenko Beam Model and DPG Method

Two possible formulations can be utilized to apply the DPG method for our problem: ultraweak or primal form. We introduce the ultraweak form in this section. Besides, we present the formulation based on trial space U and test space V.

To commence, it is not difficult to derive the first-order system corresponding to the problem (5.2), where we are seeking $\mathbf{u} = (u, \theta, \vartheta, \omega) \in U$ such that

$$\begin{aligned} \frac{\partial u_y}{\partial x} - \vartheta &= 0, \\ \frac{\partial \theta}{\partial x} - \omega &= 0, \\ -Gh\kappa(\frac{\partial \vartheta}{\partial x} - \omega) - f &= 0, \\ Gh\kappa(\vartheta - \theta) - \frac{Eh^3}{12}\frac{\partial \omega}{\partial x} &= 0, \end{aligned}$$
(5.5)

testing the first order system (5.5), with the test functions $\mathbf{v} = (v, \tau, r, q)$ and using Green's formula on a mesh $\Omega_h \subset \Omega$, and skeleton $\Gamma_h \subset \Gamma$, we obtain

$$(u_{y}, \frac{\partial v}{\partial x}) + (\vartheta, v) - \langle u_{y}, v \rangle = 0,$$

$$(\theta, \frac{\partial \tau}{\partial x}) + (\omega, \tau) - \langle \theta, \tau \rangle = 0,$$

$$(\vartheta, Gh\kappa \frac{\partial r}{\partial x}) + (Gh\kappa \omega, r) - (f, r) + \langle Gh\kappa \vartheta, r \rangle = 0,$$

$$(Gh\kappa \vartheta, q) - (Gh\kappa \theta, q) + (\omega, \frac{Eh^{3}}{12} \frac{\partial q}{\partial x}) - \langle \frac{Eh^{3}}{12} \omega, q \rangle = 0,$$
(5.6)

where (\cdot, \cdot) is the inner product in the Hilbert space U_h , and $\langle \cdot, \cdot \rangle$ is the duality pair in the Hilbert space. In the ultraweak formulation (5.6), we have no derivative of the trial variables and we assume that they are defined in $L_2(\Omega_h)$. Thus, the boundary variable of the field variables are meaningless on the skeleton Γ_n , and we introduce new trace variables $(\hat{u}, \hat{\theta}, \hat{\vartheta}, \hat{\omega})$, where the hat variables belong to the trace space $H^{-\frac{1}{2}}(\Gamma_h)$. So, if we define the group variables $\mathbf{u} = (u, \theta, \vartheta, \omega)$, $\hat{\mathbf{u}} = (\hat{u}, \hat{\theta}, \hat{\vartheta}, \hat{\omega})$, and $\mathbf{v} = (v, \tau, r, q)$ the ultraweak formulation corresponding to the system (5.2) is as follows

$$b((\mathbf{b}, \hat{\mathbf{u}}), \mathbf{v}) = -(u_y, \frac{\partial v}{\partial x}) + (\vartheta, Gh\kappa q - v + Gh\kappa \frac{\partial r}{\partial x}) + (\theta, -\theta - Gh\kappa q) + (\omega, \tau + Gh\kappa r + \frac{Eh^3}{12}\frac{\partial q}{\partial x}) + \langle \hat{u}, v \rangle + \langle \hat{\theta}, \tau \rangle + \langle \hat{\vartheta}, r \rangle - \langle \hat{\omega}, q \rangle = (f, r) = l(\mathbf{v}).$$
(5.7)

So far, we derived the ultraweak formulation (5.7) of the Timoshenko beam problem. It is well-known that using the DPG method is not practical unless we use broken (discontinuous) test space, and this will slightly alter the formulation of (5.7). Assuming a mesh \mathcal{T} , of ω including disjoint elements of $\in \mathcal{T}$, the

broken spaces $H^1(\mathcal{T})$ with the piecewise inner product $(u, v)_{\mathcal{T}} = \sum_{K \in \mathcal{T}} (u|_k, v|_k) K$, the broken ultra weak formulation seeks $(\mathbf{u}, \hat{\mathbf{u}}) \in L^2(\Omega) \times H^{-\frac{1}{2}}(\Gamma_h)$ such that

$$b((\mathbf{u}, \hat{\mathbf{u}}), \mathbf{v}) = l(\mathbf{v}) \quad \forall \mathbf{v} = (v, \tau, r, q) \in H^1(\mathcal{T}) \times H^1(\mathcal{T}) \times H^1(\mathcal{T}) \times H^1(\mathcal{T})$$
(5.8)

(5.9)

where $b(\cdot, \cdot)$ is the bilinear form and linear form $l(\cdot)$ defined as follows

$$b((\mathbf{b}, \hat{\mathbf{u}}), \mathbf{v}) = -(u_y, \frac{\partial v}{\partial x})_{\mathcal{T}} + (\vartheta, Gh\kappa q - v + Gh\kappa \frac{\partial r}{\partial x})_{\mathcal{T}} + (\theta, -\theta - Gh\kappa q)_{\mathcal{T}} + (\omega, \tau + Gh\kappa r + \frac{Eh^3}{12}\frac{\partial q}{\partial x})_{\mathcal{T}}$$

$$+ \langle \hat{u}, v_{\partial \mathcal{T}} \rangle_{\partial \mathcal{T}} + \langle \hat{\theta}, \tau_{\partial \mathcal{T}} \rangle_{\partial \mathcal{T}} + \langle \hat{\vartheta}, r_{\partial \mathcal{T}} \rangle_{\partial \mathcal{T}} - \langle \hat{\omega}, q_{\partial \mathcal{T}} \rangle_{\partial \mathcal{T}}$$
$$l(\mathbf{v}) = (f, r)_{\mathcal{T}}$$

It is proven [21, 13] that the form (5.8) is well-posed, that is, the discrete stability is guaranteed independently from choosing a mesh. Now, we can discretize the ultraweak form with the DPG method using optimal test space. The theory behind the DPG method using optimal test space and numerical implementation of this method will be presented in the section. But, we vaguely move toward different steps of implementing the DPG method in the proceeding of this section.

Let's start with the fact that the DPG method significantly depends on the choice of the test space inner product since it determines the norm in which the DPG method is optimal. As an illustration, if the errors in L_2 -norm are of interest, there is a tangible theory [21] that shows that the graph norm is a suitable choice for the test space. In this work, we propose the following graph norm

$$\|\mathbf{v}\|_{V} = \|(v,\tau,r,q)\|_{V} = \|\frac{\partial v}{\partial x}\|_{L_{2}} + \|Gh\kappa q - v - Gh\kappa\frac{\partial r}{\partial x}\|_{L_{2}} + \|\frac{\partial \tau}{\partial x} - Gh\kappa q\|_{L_{2}} + \|-\tau + Gh\kappa r + \frac{Eh^{3}}{12}\frac{\partial q}{\partial x}\|_{L_{2}}.$$

$$(5.10)$$

The analysis of this graph norm and the exact procedure for finding it will be discussed in the section thoroughly. Having the graph norm and as a direct result the inner product of the test space, we are ready to discretize the ultraweak form and construct the DPG system.

In the classical Galerkin method, the convention is to choose the same discrete space for both trial and test spaces, so a squared linear system is expected. However, in the DPG method, discrete trial $U_h \subset U$ and test space $V_h \subset V$ have different dimensions. The practical DPG method with optimal test space benefits from enriched test space, meaning that dim $V_h \ge \dim U_h$. We assume that $\{u_j\}_{j=1}^N$, and $\{v_j\}_{j=1}^M$ are the bases of trial and test spaces respectively where $M \ge N$. In the DPG methodology, each trial space basis function u_i and corresponding optimal test function v_i^{opt} satisfy the following system

$$(v_i^{\text{opt}}, \delta v)_V = b(u_i, \delta v), \quad \forall \delta v \in V$$
 (5.11)

Now let's define $M \times M$ Gram matrix $G = (G_{ij})_{M \times M}$

г

$$G_{ij} = (v_i, v_j)_V$$

and $N \times M$ stiffness matrix $B = (B_{ij})_{N \times M}$

$$B_{ij} = b(u_i, v_j)$$

where the *B* has the following structure

$$B = \begin{bmatrix} B_{uv} & B_{\theta v} & B_{\theta v} & B_{\omega v} & B_{\hat{u}v} & B_{\hat{\theta}v} & B_{\hat{\theta}v} & B_{\hat{\omega}v} \\ B_{u\tau} & B_{\theta\tau} & B_{\theta\tau} & B_{\omega\tau} & B_{\hat{u}\tau} & B_{\hat{\theta}\tau} & B_{\hat{\theta}\tau} & B_{\hat{\omega}\tau} \\ B_{ur} & B_{\theta r} & B_{\theta r} & B_{\omega r} & B_{\hat{u}r} & B_{\hat{\theta}r} & B_{\hat{\theta}r} & B_{\hat{\omega}r} \\ B_{uq} & B_{\theta q} & B_{\vartheta q} & B_{\omega q} & B_{\hat{u}q} & B_{\hat{\theta}q} & B_{\hat{\theta}q} & B_{\hat{\omega}q} \end{bmatrix}_{N \times M}$$

$$(5.12)$$

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and *l* the mass matrix l(v) = (f, r). We use high order Lagrange basis of different order to expand the trial space with order *P*, and enriched test space with order $p + \Delta p$ for $\Delta p = 1, 2, \cdots$. The global assembly will have the following form

$$B^{\text{n-op}}\mathbf{u}_h = B^T G B \mathbf{u}_h = B^T G^{-1} l = l^{\text{n-op}}$$
(5.13)

It is worth noting that thanks to the broken structure of the test space, evaluating optimal test functions in the Gram matrix and its inversion are localized and therefore the global assembly can be parallelized, which makes the DPG method a practical method to solve the beam problem.

5.4 Numerical Experiments

In this section, we showcase the solution of problem (5.2) when f = 1. we use the Lagrange polynomial basis of degree p = 1, 2 for discretizing the trial space and we used the broken enriched test space with $\Delta p = 2$.



Figure 5.1: Left hand side is deflection of model and right hand side is the rotation of them model approximated by DPG method with trial space of order p = 1.

Figures (5.1), (5.2), and (5.3) illustrates the result for implementation of Timoshenko beam model with supported and supported boundary conditions of thickness $t = e^{-4}$, for Lagrange basis functions of order p = 1, 2, 3. I used the uniform mesh of including 16 elements. As, it can be seen from figures the method is robust specially for small thickness.



Figure 5.2: Left hand side is deflection of model and right hand side is the rotation of them model approximated by DPG method with trial space of order p = 2.



Figure 5.3: Left hand side is deflection of model and right hand side is the rotation of them model approximated by DPG method with trial space of order p = 3.

CHAPTER VI

CONCLUSIONS

In this dissertation presents an exploratory study of variational inequalities, their solution approaches and sensitivity analysis formulation. The literature on this topic is extensive with fundamental contributions coming from the applied mathematics community. The engineering community has been solving variational inequalities in the form of contact problems and those with elastoplastic material behavior. However, the mathematical nuances of the formulation and its relations with related forms of variational inequalities are absent from the engineering literature. This paper is our effort to build a clearer understanding of these relations.

This work investigates approaches to solve two different types of variational inequalities in onedimension: a contact problem that places bounds on the solution variable, and a problem with elastoplastic material that requires that the stress and internal variables satisfy the inequality placed by a yield criterion. These problems are simple in nature, but include all complexities of any large-scale finite-dimensional problem of a similar form. Therefore, the solution approaches presented here will be applicable to higher dimensional problems with suitable modifications to address scalability of the solvers.

The contact problem has been solved using a minimization approach and a complementarity approach. The former requires a minimization statement for the problem, which, for example, is readily available for problems in mechanics in the form of the principle of total minimum potential energy, and the principle of maximum dissipation for elastoplastic problems. Once stated in a minimization form, additional constraints can be easily added to the problem statement. Large-scale problems can be solved using efficient interiorpoint methods or using primal-dual algorithms. The complementarity solver can efficiently handle nonlinear problems with bound constraints on solution variables.

The elastoplastic problem is converted using the projection method from a primal-mixed variational inequality to a primal variational equality that is solved using a semi-smooth Newton solver. Sensitivity analysis formulation for this form has been demonstrated.

Ongoing work is exploring similar problems in two- and three-dimensional domains with numerical solution obtained using these approaches. Additionally, the details of formulating and implementing the other equivalent forms of the variational inequalities, namely Weiner-Hopf equation, fixed-point problem and primal-dual solution of plasticity problem are being investigated.

Focusing on designing stable numerical scheme for problems that violate coercivity, finite element analysis of the problem of the migration risk problem is comprehensively studied and different theoretical and numerical properties of the proposed numerical scheme are explored. We showed that classic finite element method can be used to numerically solve the free boundary value problem arisen form the migration rate problem in credit risk study. The proposed variational form proposed in this paper is well-posed, that is the solution driven from this form is bounded. Analysis result about corresponding elliptic form of the problem assist in deriving convergence result for the numerical method for the free boundary value problem, although our estimates in this investigation are not always sharp. Benefiting form properties of adjoint problem and Green function, a direct method is devised to estimate the free boundary value problem. Numerical results showcased the quality of the proposed numerical methodology, and we saw better result in high order Lagrange finite element. in this work we assess the Backward Euler scheme, we may extend the method to the Crank-Nikolson scheme as well. The complexity and heavy theoretical work done for this section showed that designing a stable and well-posed numerical scheme for a problem that has the potential of coercivity loss can be a tedious task. Thus, the Discontinuous Petrov Galerkin (DPG) method with the optimal test space as an alternative is studied in this investigation to tackle the coercivity loss. The DPG method is proposed for a wide range of problems in quantitative finance including pricing vanilla and exotic options. Besides, the numerical characteristic of this method is illustrated numerically with a thorough analysis of the whole family of those problems. This method is also used for Elastic bending analysis of very thin beams, and the results show that the method is accurate and robust. Moreover, a review of variational inequalities as the principal tool in optimization theory for studying free boundary value problems such as exotic option pricing and plasticity problems in mechanics, and a novel adjoint sensitivity analysis of the variational inequalities are proposed for the first time is provided.

6.1 Contributions

The contribution of this dissertation is as following

- Proposing a stable Finite element method and analysis of Migration risk problem
- Designing the adjoint sensitively of variational inequalities
- Proposing DPG method for elastic analysis of very thin beam theory
- Proposing the DPG method for the first time in quantitative finance for pricing a broad family of exotic and vanilla options
- Developing high-performance code for DPG method in quantitative finance

6.2 For Further Research

This investigation paved the way for using the powerful DPG method in other sensitive and complicated problems in quantitative finance. Developing the DPG method for the option pricing under a more realistic model, the jump-diffusion model, is a potential future research problem. In computational mechanics fields, developing DPG method for elastic bending and vibration analysis of composites of materials based on

layer-wise theory is under preparation and due to the application of composites in designing more efficient vehicles, this field can be explored more thoroughly in the future. Analysing DPG method for nonlinear analysis of the elastoplastic problem is another area of research that can be investigated.

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