MULTISCALE FINITE ELEMENT METHOD FOR PDE CONSTRAINED OPTIMIZATION IN HIGH GRADIENT PROBLEMS

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DEDICATION

This thesis is dedicated to my wife Adekemi, our son Emmanuel and my mother, Chief (Mrs) C.O Akeremale for their undeniable love and sacrifices.

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ABSTRACT

A multiscale finite element method (MsFEM) was introduced for high gradient Partial Differential Equation (PDE) constrained optimization problem. Starting with the traditional fournode finite element method, additional nodes were inserted automatically at high gradient regions by an adaptive algorithm based on refinement criteria. A posteriori error estimation and error indicator were formulated. The error estimation was residual-based, while the error indicator was gradient-based. Using the information from the gradient-based error indicator, a p-refinement indicator was used to decide whether a given element should be refined or not via adaptive algorithm. Two sets of elements were used to design the adaptive algorithm: the regular elements and transition elements. The regular elements are the linear and quadratic elements, while the transition elements are the elements having both quadratic and linear sides, useful in transitioning from linear to quadratic elements during the implementation of the adaptive algorithm. The coupling resulted in a MsFEM. An exact solution containing high-gradient and multivariate polynomial functions that satisfies the PDE constraint and minimizes the objective function was also created using MAPLE software. A PDE constrained error analysis was also developed and implemented. The proposed MsFEM was applied to PDE constrained optimization problem with localised high gradient to analyse and validate the performance and accuracy of the proposed technique. The obtained numerical results from the analysis in terms of relative error showed an encouraging and promising performance of the scheme. The numerical results showed that the technique could help in solving high gradient problems with accuracy and minimum error.

ABSTRAK

Kaedah elemen terhingga berbilang skala (MsFEM) telah diperkenalkan untuk masalah pengoptimuman kekangan Persamaan Pembezaan Separa (PDE) berkecerunan tinggi. Bermula dengan kaedah unsur terhingga empat nod tradisional, nod tambahan telah dimasukkan secara automatik pada kawasan kecerunan tinggi melalui algoritma penyesuaian berdasarkan kriteria penghalusan. Anggaran ralat posterior dan penunjuk ralat telah dirumuskan. Anggaran ralat adalah berasaskan kaedah baki, manakala penunjuk ralat adalah berasaskan kecerunan. Menggunakan maklumat daripada penunjuk ralat berasaskan kecerunan, penunjuk penghalusan-p digunakan untuk memutuskan sama ada unsur tertentu perlu diperhalusi atau tidak melalui algoritma penyesuaian. Dua set unsur telah digunakan untuk mereka bentuk algoritma penyesuaian: unsur biasa dan unsur peralihan. Unsur biasa ialah unsur linear dan kuadratik, manakala unsur peralihan ialah unsur yang mempunyai kedua-dua sisi kuadratik dan linear, berguna dalam peralihan daripada unsur linear kepada kuadratik semasa pelaksanaan algoritma penyesuaian. Gandingan ini menghasilkan MsFEM. Penyelesaian tepat yang mengandungi fungsi polinomial kecerunan tinggi dan multivariat yang memenuhi kekangan PDE dan meminimumkan fungsi objektif juga dicipta menggunakan perisian MAPLE. Analisis ralat terhalang PDE juga dibangunkan dan dilaksanakan. MsFEM yang dicadangkan telah digunakan untuk masalah pengoptimuman terhad PDE dengan kecerunan tinggi setempat untuk menganalisis dan mengesahkan prestasi dan ketepatan teknik yang dicadangkan. Keputusan berangka yang diperoleh daripada analisis dari segi ralat relatif menunjukkan prestasi skim yang memberangsangkan dan menjanjikan. Keputusan berangka menunjukkan bahawa teknik ini dapat membantu menyelesaikan masalah kecerunan tinggi dengan ketepatan dan ralat yang minimum.

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LIST OF ABBREVIATIONS

AFEM	-	Adaptive Finite Element Method
CFD	-	Computational Fluid Dynamics
D	-	Dirichlet
DB		Dirichlet Boundary
debc	-	Dirichlet boundary condition
df	-	Neumann boundary condition
FE	-	Finite element
FEM	-	Finite Element Method
HG	-	High Gradient
h-refined	-	Mesh-refined
IPM	-	Interior Point Method
ℵ	-	Set of all nodes
I	-	Interior nodes
IN	-	Internal + Neumann nodes
KKT	-	Karush-Kuhn Tucker
LRE	-	Linear Relative Error
LtoG	-	Local to Global
MBCs	-	Mixed Boundary Conditions
MsFEM	-	Multiscale Finite Element Method
MsRE	-	Multiscale Relative Error
NAND	-	Nested Analysis and Design
NBD	-	Neumann Boundary Condition
NHG	-	Non-High Gradient
NAND	-	Nested Analysis and Design
NBD	-	Neumann Boundary Condition
NHG	-	Non-high gradient
ODEs	-	Ordinary Differential Equations
p-AFEM	-	Polynomial adaptive finite element method MsFEM
PDEs	-	Partial Differential Equations
PDECO	-	PDE Constrained Optimization

p-refined	-	Polynomial-refined
SAND	-	Simultaneous Analysis and Design
SNL	-	Sandia National Laboratory
SQP	-	Sequential Quadratic Programming

LIST OF SYMBOLS

K	-	Global stiffness matrix
k	-	Elemental stiffness matrix
β	-	Regularization parameter
p	-	Polynomial
h	-	Mesh
i	-	Row
j	-	Column
∇	-	Gradient (nabla)
J^{-1}	-	Jacobian inverse
J^{e}	-	Jacobian
Γ	-	Boundary
Γ_D	-	Dirichlet Boundary
Γ_N	-	Neumann Boundary

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CHAPTER 1

INTRODUCTION

1.1 Problem Background

This chapter addresses the two topics relevant to this work: optimization, partial differential equations (PDE). The main emphasis of this work is the application of multiscale technique for two-dimensional PDE constrained optimization problems. Therefore, an overview of the two topics, background, problem statement, research objectives, research questions, scope, and significance of the research are discussed in this chapter.

1.2 Background

Optimization is a fundamental instrument in the investigation of actual physical systems and could be characterized as the science of determining the best arrangement among every possible answer for a specific mathematical concern. Engineers must make decisions in constructions, designs, and even maintenance, and such choices are to either maximize gains or minimize efforts. These gains or efforts are often expressed as a function of certain design variables. Computational methods and solution procedures for optimization problems are selected based on the classification of the problems (constrained or unconstrained optimization problems). Figure 1.1 showcase a graphical representation of the characterization of optimization problems with specific spotlight on PDE constrained.

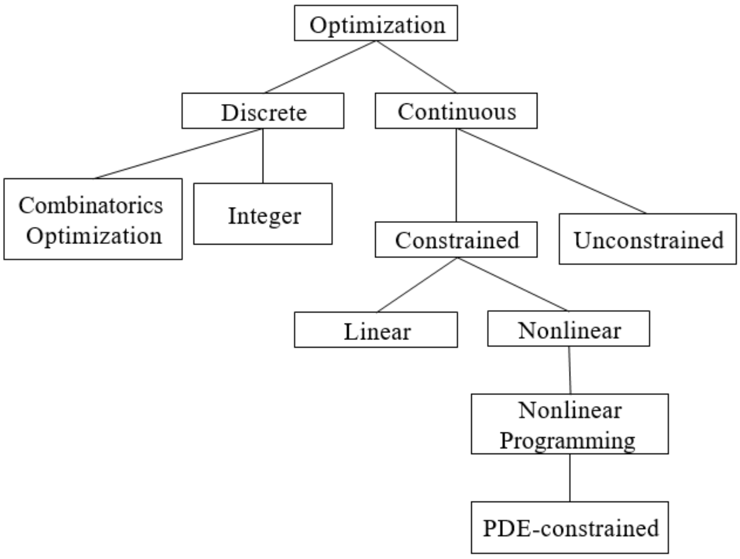

Figure 1.1: Classification of optimization problems

1.2.1 PDE Constrained Optimization Problems

PDEs are generally used to model physical phenomena, and the solution to such problems poses a serious challenge, especially where the problem is complex and exact solution does not exist. There are many problems in physics, chemistry, mechanics, finance, biology, engineering, and other fields that involve complex systems. These include elasticity, plastic, fluid flow, quantum mechanics, electrodynamics, acoustic and heat transfer (Peinke *et al.* 2019); (Aliev *et al.* 2018); (Fowler *et al.* ;2019); (Chernikov 2017); (Khan *et al.* 2019); (Liu 2018); (Fang *et al.* 2019); (Casati *et al.* 2020); (Brezis and Browder 1998); (Phong 2019); (Arrigo 2019); (Collins, 2019). Often, modelling of such complex systems results in solving PDEs. The general form of PDEs with two independent variables, according to (Zhang and Khalique 2018) is given in Equation (1.1).

$$F\left(x, y, u(x,y), u_x(x,y), u_y(x,y)\right) = F\left(x, y, u, u_x, u_y\right) = 0. \tag{1.1}$$

Mathematically, PDEs represent an ample range of common logical occurrences, and in turn, applications in engineering and life sciences ubiquitously give rise to problems formulated as PDE-constrained optimization (PDECO) problems as shown in Equation (1.2), (Stoll and Breiten 2015); (Zhang and Zhang 2011); (Al-Smadi *et al.* 2017); (Tariq and Seadawy 2017); (Ruthotto and Haber 2018). A PDE-constrained optimization (PDECO) problem is a modelled used to find the optimal solution satisfying its PDE constraints, boundary conditions and the objective function. PDECO problems arise in such diverse areas as environmental engineering, aerodynamics, and medicine (Salmoiraghi *et al.* 2018); (Hammad *et al.* 2020); (Gkaragkounis *et al.* 2020). The solution to PDE-constrained optimization problems are naturally challenging considering the PDE constraint but for the advancement in optimization techniques and increase in the power of computing as evident in PDE solvers and many of which have been studied in recent times by (Antil *et al.* 2018); (Leithäuser *et al.* 2018); (Kaercher *et al.* 2018); (Herzog *et al.* 2018); (Hintermüller *et al.* 2018); (Mang *et al.* 2018). The general form of PDE-constrained optimization problem is as shown in Equation (1.2) below.

$$\begin{aligned} &\min_{u,q} f(u,q) \\ &\text{s.t. } c(u,q)=0 \end{aligned} \tag{1.2}$$

where $f(u,q)$ is the functional (objective function) and $c(u,q)$ represents the differential operator, u is the state variable and q is the control variable.

PDECO is a relatively young and rapidly developing area of research. PDECO problem is applicable in flow simulation (see Figure 1.2), PDECO tries, for example, to minimize fuel consumption, in order to optimize flight trajectory, or to minimize manufacture cost. Also, in Figure 1.3 (elastic deformation), PDECO attempts to optimize material strength in order to reduce production expenses, or to optimize its stress under heavy loads. In thermal control, PDECO is used to optimize the temperature of an object, for example, an optimal component's temperature will result in optimal performance in electrical devices. In electric cars, PDECO is used to extend battery life span Alqarni. PDE-constrained optimization (PDECO) problems also occur in various fields, like atmospheric and oceanic sciences (variational data assimilation) to predict the weather for several days, in medical image analysis (image registration) to find point-wise correspondences between images, in mathematical finance (inverse problem of option pricing), in shape optimization and thermal control (optimal heat control) Alqarni (2019). The most classical PDE constrained optimization problems emerge in the context of design and control of engineering systems. These problems promise to deliver engineering systems with superior performance than otherwise possible. They will have the greatest impact in highly complex situations where intuition breaks down and experimentation are expensive, difficult, or dangerous (Zahr, 2016); (Qian *et al.* 2017). The design and state variables of these problems all exhibit large numbers.

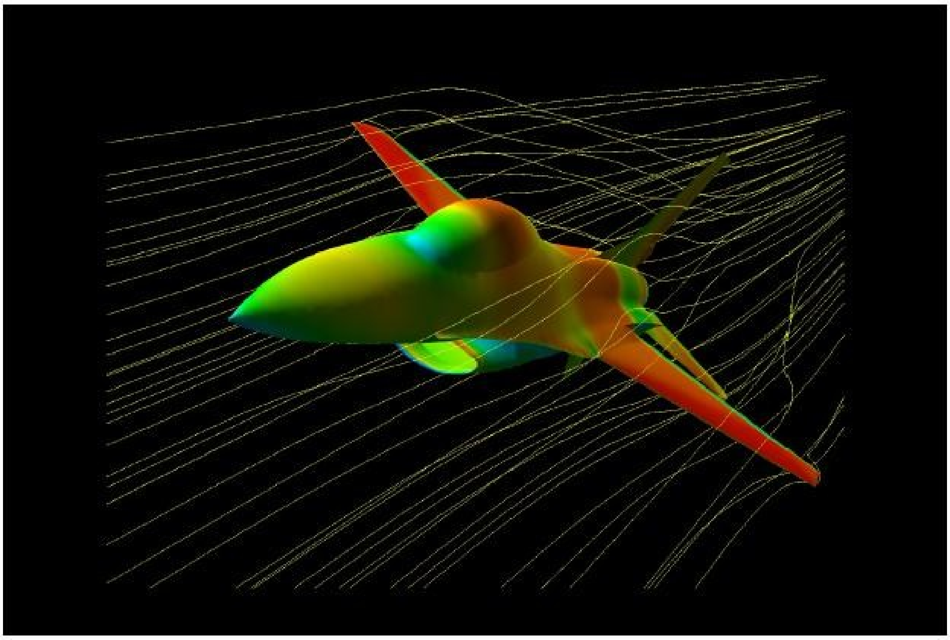

Figure 1.2: Mach contours and streamlines for an aeroelastic simulation on the surface of an aircraft at Mach 0.9 Alqarni (2019)

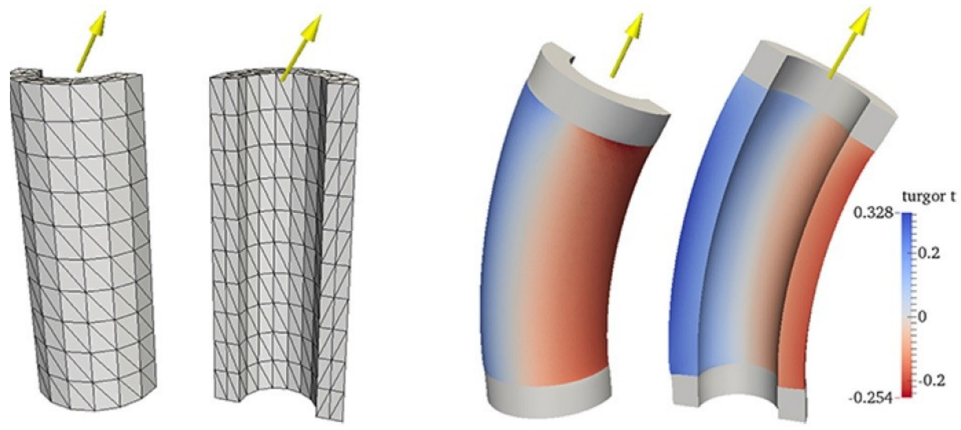

Figure 1.3: The front and back of a stem before and after applying a force to get the desired shape (Alqarni, 2019)

According to (Alqarni, 2019), PDECO problems are significant because they occur in various fields, for example, in atmospheric and oceanic sciences (variational data assimilation) to predict the weather for several days (Qiu *et al.* 2018), in medical image analysis (image registration) to find point-wise correspondences between images, in mathematical finance (inverse problem of option pricing) (Karatzas *et al.* 1998), in shape optimization, (He *et al.* 2019) and thermal control (optimal heat control). PDE constrained problem can also be an automatic parameter searching in which organized computational arrangement replaces interactively modify-and-try iterations. While an objective function is designed to represent the goal, the aim is to know the PDE parameter that gives an optimum (a minimum) (Neitzel *et al.* 2019). Most often, the objective is dependent on just the PDE's solution, the state variable that indirectly can be affected by the changes of the control variable q through the PDE constraint Huber (2013). It is established in many applications of PDE constrained optimization problems based on the way the PDE parameters influence the state variables (Huber, 2013); (Choi, 2012).

In shape optimization, one tries to optimize some functional quantity (e.g., drag or lift of a wing) by varying the shape of an object (e.g., a wing or a car). The pump of arteries in medicine is also an example of shape optimization, and the aim is to minimize the shear rate to avoid thrombus formation or red blood cell damage at the device surfaces (Huber 2013). The governing equations in most examples in this class of PDE-constrained optimization problems are non-linear Navier-Stokes equations.

Inequality constraints prevent substantially trivial parameter settings, such as a very small wing sweep angle or a negative local mass for a structural element. Shape optimization has also been used in biological applications, e.g., to design the shape of the incoming branch of the aorta-coronary bypass (Zahr, 2016).

In inverse problems or parameter identification, the aim is to find properties of a substantial structure based on a given analysis. To solve an inverse problem is the aim of parameter estimation. In this problem set, the idea is to seek PDE parameters, called the model, that are very logical with analysis. The parameters (usually material parameters) affect the differential operator, and solving such problems is generally more difficult than optimal control problems. Most medical image methods are based on inverse problems. For example, in tomography, electrical impedance, to mention a few, the body's surface is being supplied current. An electrical capacity that depends on the heat inside the body is developed. The location-dependent heat is considered a PDE parameter varied to minimize the difference between actual analysis value and simulation value. The same approach can be applied in direct current (DC) resistivity assessment and groundwater modelling (Huber 2013).

1.2.2 High Gradient Problems

High-gradient problems are problems that exhibit rapid changes or sharp fronts or wiggles in their numerical solutions. Wiggles are spurious node-to-node oscillations affecting solutions and are vital since they usually harbour remarkable physical phenomena such as shock formulations, turbulence, and boundary layers and typically localised (Gresho and Lee, 1981). Advection-dominated problems which naturally occur in fluid dynamics can be considered a high gradient problem. These problems commonly exhibit high gradients near domain boundaries (boundary layers) and inside the domain (shocks).

It is typically necessary to stabilize the standard FEM in order to keep away from spurious oscillations in the high gradient region (Abbas *et al*., 2010). It has been shown that even with stabilization, high gradients are insufficiently represented accurately on coarse meshes. Thus, the only way to eliminate problems like this is to severely refine the mesh, such that convection no longer dominates on an element level.

1.3 Types of PDE Constrained Optimization

Different types of PDECO exist, and this depends on how the PDE parameters affect the state variable. Since the PDE is the constraint to the function to be minimized, and it also plays a significant role in the numerical solution of the PDECO, it is vital to examine the class of the problem by stating the type of PDE constrained problem and the PDE, which are typically solved. Both the objective function and the constraint (PDE) can be of the same type as linear, nonlinear, time-dependent, time-independent, or different types. However, in this study, we focus on a quadratic time-independent objective function and time-independent linear PDE as a constraint.

1.3.1 Distributed Control Problem

A PDE-constrained problem in which the control is applied over the entire domain is a distributed control problem as shown in Equations (1.3) and (1.4) below. However, PDE constrained optimization problems are not restricted to this.

Consider the PDE constrained below,

$$\min_{u,q} \frac{1}{2}\int_{\Omega} \left(u-\overline{u}\right)^2 d\Omega + \frac{\beta}{2}\int_{\Omega} q^2 d\Omega \tag{1.3}$$

subject to:

$$\left.\begin{aligned} -\nabla^2 u &= q, \quad \Omega \\ u &= g, \quad \partial\Omega_D \end{aligned}\right\} \tag{1.4}$$

where, q, u represent the control and state variables respectively, $\bar{u}$ is the given target or desired variable, $\beta > 0$ is the regularization parameter (Tikhonov parameter) added to functional to avoid ill-conditioning, g is the Dirichlet boundary condition. The state variable and control variables belong to space of twice differentiable functions $\left(u \in C^2(\Omega)\right)$ and $\left(q \in C^2(\Omega)\right)$, (Hinze *et al.,* 2008).

Theoretically, when the significant addition of control into the system is penalized, it could be to make the state and the desired variables very close. for this type of problem, In physical term or real situation, this may be seen as penalizing the energy input into such system Figure and (Stoll 2013); (Pearson *et al.* 2012); (Pearson *et.al* 2020). The state variable can be light intensity, temperature, humidity, or a combination of these parameters. The energy put into the system to achieve the desired variable or conditions could be the control variable. The PDE could be heat equation or an equation of a similar structure in the problem set-up.

1.3.2 Boundary Control Problem

It is imperative to know that besides the distributed control problem discussed above, subdomain and Neumann boundary control problems are mentioned below.

Consider

$$\min_{u,h} \frac{1}{2}\int_{\Omega} (u-\bar{u})^2 \, d\Omega + \frac{\beta}{2}\int_{\Gamma} q^2 d\Gamma \tag{1.5}$$

Subject to:

$$\left.\begin{aligned} -\nabla^2 u &= h, \quad \Omega \\ \frac{\partial u}{\partial n} &= q, \quad \partial\Gamma \end{aligned}\right\} \tag{1.6}$$

where, q, u represent the control and state variables respectively, h is the source term and $\bar{u}$ is the target or desired variable, $\beta > 0$ is the regularization parameter (Tikhonov parameter) added to functional to avoid ill-conditioning. The state variable and control variables belong to space of twice differentiable function $\left(u \in C^2\left(\Omega\right)\right)$ and $\left(q \in C^2\left(\partial\Omega\right)\right)$, (Hinze *et al.,* 2008).

Contrary to distributed control problem as mentioned above, control is enforced at the boundary in this case. This class of problem is more practical and realistic in real-life situations, especially in any application that has to do with flows because the boundary might be the only physical feature open to control. The main class of this problem is Neumann boundary control. It implies that the control is applied to the PDE like natural boundary conditions. The penalized term on the control, rather than being measured as an integral over the whole domain, is now measured as a boundary integral. In solving such a problem numerically, it is logical to seek for discretization scheme like the Finite Element Method that can handle both regular and irregular geometries. Also, the state variable and the control variable must consist of different shape functions corresponding to the boundary alone and the entire domain, respectively.

1.3.3 Subdomain Control Problems

The subdomain control problem is another class of PDECO, in which the matrix structure is like that of boundary control problems. In this class of problem, control is enforced on the interior subdomain Ω_{sub} of the domain Ω. It happens where only parts of the domain can be controlled. For example, it is natural, in a flow, for the entry region of the domain to be subjected to control. For Poisson's equation, the Subdomain control problem can be written as

$$\min_{u,q} \frac{1}{2}\int_{\Omega} \left(u-\bar{u}\right)^2 d\Omega + \frac{\beta}{2}\int_{\Omega} q^2 d\Omega \tag{1.7}$$

Subject to:

$$-\nabla^2 u = \begin{matrix} q, & \Omega_{sub} \subset \Omega \\ 0, & \Omega \setminus \Omega_{(sub)} \end{matrix} \Bigg\} \quad (1.8)$$

Though the system formulation of the problem shows that the control may only be enforced on the subdomain Ω_{sub}, but there is a need to control the quantity $(u - \bar{u})$ on the whole domain Ω.

1.4 Problem Statement

It is well known that problems can be solved for practical and effective interpretation if they can be represented mathematically. Nowadays, PDE constrained optimization problem is one of the significant ways that real-life problems are modelled and represented.

Mathematical optimization problems govern a significant number of important and challenging applications in mathematics as well as engineering. One important class of these problems that have broad applications in virtually all fields of human endeavours like biological mechanisms and chemicals, fluid flow, and medical imaging is PDE constrained optimization (PDECO). Though such problems can typically be written precisely, generating correct numerical solutions to such problems where the PDEs are of the high gradient is a very non-trivial task. Moreover, it is time-consuming and computationally expensive due to the size and complexity of the resulting system of equations.

Considering the above, this research develops a robust and accurate multiscale technique coupled with finite element method (multiscale method) that detects the region of high gradient through automation for proper discretization without sacrificing any component of the problem, thereby reduce the cost of computation of the generated linear system.

1.5 Research Questions

Consider the peculiarity of the two different areas of research in this study (PDE and Optimization), as stated in Equations (1.3) and (1.4), the following questions are raised

1. How can a numerical method detect the high gradient area automatically in a domain of interest?
2. How to create a numerical procedure to solve the PDE Constrained optimization problem in high gradient?
3. Is the PDECO problem well-posed?
4. Does the solution converge?

1.6 Research Objectives

The primary aim of this study is to develop adaptive multiscale finite element method that will enhance solution to PDE constrained optimization problem in high gradient. The following are the main objectives to achieve the goal:

1. To develop a p-adaptive multiscale finite element method (AFEM) by applying automation of critical region detection.
2. To apply p-adaptive multiscale finite element method (AFEM) to PDE Constrained optimization problem.
3. To design a well posed test problem to be used in the assessment of the viability of the proposed method.
4. To provide a method for the calculation of assessment error.

1.7 Scope of the Research

Several method of discretization exit in literature, however, this study focuses on p-adaptive multiscale finite element method for solving PDE constrained optimization problems. The formulation and application of the anticipated new technique is restricted to high gradient problems in two-dimension and Poisson equation. The tools used to compute the numerical results are codes written in MAPLE and OCTAVE programming languages. OCTAVE been a free software is used for the simulation.

1.8 Significance of the Research

Most of the previous studies on adaptive finite element for PDE constrained optimization considered the h-adaptive finite element for PDE constrained optimization. This created a gap in the study and application of p-adaptive finite element in PDE constrained optimization. To bridge the gap, this work is based on formulating a p-adaptive finite element for PDE constrained optimization. The work is premised on the qualities of p-adaptive algorithm which are: (i) better conditioned matrices; (ii) required no alteration of the mesh and can easily be used in the adaptive analysis (iii) can predict accurate solutions for a simple structure; (iv) tend to give the same accurate results with far fewer degrees of freedom (DOF) than the h-version; (v) can overcome some locking problems; and (vi) have less program challenges compare to hp-version (Leung, 2007). The proposed p-adaptive finite element envisaged as the research outcome, can produce higher precision results. This makes it a veritable technique for solving high gradient PDE constrained optimization problems. In addition, the outcomes can stimulate new gaps that can be leveraged upon for further research in related areas.

1.9 Summary and Organization of the Thesis

The work consists of six chapters, and the chapters are arranged as follows: Chapter 1 presents the problem's background, followed by the statement of the problem, research questions, and study objectives. Also, the scope and significance of the study is stated. Finally, the format of the thesis is established.

Chapter 2 presents a comprehensive review of earlier studies on the numerical techniques for PDE-constrained optimization problems and the research gap

Chapter 3 captured the detailed description of finite element method (FEM) and multiscale technique (the p-adaptive finite element method (p-AFEM)), the error estimation and the selection of the high gradient region to achieve the research objectives. The validation techniques and robust residual error analysis theorem based on matrix condition numbers are discussed.

Chapters 4 entails the formulation of linear system from distributed PDE constrained optimization problem. Also exact solution in polynomial form that satisfies both the PDE constraint and minimize the objective function was created using MAPLE software. The Objective value and PDECO error analysis were also discussed.

Chapters 5 give the numerical performance of the proposed multiscale technique as discussed in chapter 3. Compare the proposed method with traditional finite element method in terms of error and confirms the convergence of the error and the objective value of the proposed method.

Lastly, in Chapters 6, the conclusions are drawn and the recommendations for future and further research illustrated.

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