

MULTISCALE HYBRID FINITE ELEMENT AND FINITE VOLUME METHOD  
FOR HIGH GRADIENT BOUNDARY VALUE PROBLEMS

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## **DEDICATION**

This thesis is dedicated to my lovely daughter,  
OLAIJU ABIMBOLA LOIS.

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## ABSTRACT

A multiscale hybrid finite element and finite volume method (MSHFEFVM) was introduced for high gradient boundary value problems by coupling an adaptive finite element and node centred finite volume schemes. Starting with the traditional four-node 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 which are 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. These elements are useful in transitioning from linear to quadratic elements during the implementation of the adaptive algorithm. The coupling resulted in a multiscale finite element method (MSFEM). The MSFEM was applied to some two-dimensional high gradient problems with promising results. The MSFEM was extended to solve the time dependent partial differential problems. The results obtained showed good agreement with the analytical results. A node centred finite volume method was coupled with the MSFEM to form a MSHFEFVM based on concurrent continuum-continuum coupling using a handshake coupling technique that allows information passing between the two coupled methods on a fly. The proposed hybrid technique was first applied to some two-dimensional localised high gradient problems with available analytical solutions. This application was necessary to analyse and validate the performance and accuracy of the MSHFEFVM. The obtained numerical results from the analysis in terms of error and execution time showed an encouraging performance of the scheme compared to the traditional finite element, the node centred finite volume and the MSFEM. Finally, the MSHFEFVM was applied to two standard localised high gradient problems and two engineering problems, which are electrostatics and torsion problems. The application showed a promising performance of the new scheme. The numerical results show that the combination of these two techniques can help to solve high gradient problems with accuracy and minimum execution time.

## ABSTRAK

Unsur terhingga hibrid multiskala dan kaedah isipadu terhingga (MSHFEFVM) diperkenalkan untuk menyelesaikan masalah nilai sempadan berkecerunan tinggi dengan menggandingkan unsur terhingga secara adaptif dan skema isipadu terhingga berpusat pada nod. Bermula dengan kaedah unsur terhingga empat nod tradisional, nod tambahan dimasukkan secara automatik di kawasan kecerunan tinggi oleh algoritma adaptif berdasarkan kriteria penyempurnaan. Anggaran ralat posteriori dan penunjuk ralat dirumuskan. Anggaran ralat adalah berdasarkan sisa, sementara penunjuk ralat berdasarkan kecerunan. Menggunakan maklumat dari penunjuk ralat berdasarkan kecerunan, penunjuk penambahbaikan  $p$  digunakan untuk memutuskan sama ada elemen tertentu harus diperhaluskan atau tidak melalui algoritma adaptif. Dua set unsur digunakan untuk merancang algoritma adaptif iaitu unsur biasa dan unsur peralihan. Unsur biasa adalah unsur linear dan kuadratik, sementara unsur peralihan adalah unsur yang mempunyai sisi kuadratik dan linear. Semua unsur ini berguna dalam peralihan dari unsur linear ke kuadratik semasa pelaksanaan algoritma adaptif. Gandingan ini menghasilkan kaedah unsur terhingga multiskala (MSFEM). MSFEM diterapkan pada beberapa masalah kecerunan tinggi dua dimensi dengan keputusan yang memuaskan. MSFEM diperluas untuk menyelesaikan masalah pembezaan separa yang bersandar pada masa. Keputusan yang diperoleh menunjukkan persetujuan yang baik dengan hasil analisis. Kaedah isipadu terhingga berpusat pada nod digandingkan dengan MSFEM untuk membentuk MSHFEFVM berdasarkan gandingan kontinum-kontinum serentak menggunakan teknik gandingan jabat tangan yang membolehkan maklumat disampaikan antara kedua-dua kaedah terganding dengan cepat. Teknik hibrid yang dicadangkan pertama kali diterapkan pada beberapa masalah berkecerunan tinggi dua dimensi yang disetempatkan dengan penyelesaian analisis yang tersedia. Aplikasi ini diperlukan untuk menganalisis dan mengesahkan prestasi dan ketepatan MSHFEFVM. Keputusan berangka yang diperoleh dari analisis dari segi ralat dan masa pelaksanaan menunjukkan prestasi skema yang memberangsangkan berbanding dengan unsur terhingga tradisional, isipadu terhingga berpusat dan MSFEM. Akhirnya, MSHFEFVM diaplikasikan pada dua masalah kecerunan tinggi yang disetempatkan dan dua masalah kejuruteraan, iaitu masalah elektrostatik dan kilasan. Pengaplikasian ini telah menunjukkan prestasi skema baharu yang memberangsangkan. Keputusan berangka menunjukkan bahawa gabungan kedua-dua teknik tersebut dapat membantu menyelesaikan masalah kecerunan tinggi dengan tepat dan masa pelaksanaan minimum.

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## LIST OF ABBREVIATIONS

FEM	-	Finite Element Method.
FVM	-	Finite Volume Method.
MSFEM	-	Multiscale Finite Element Method.
MsFVM	-	Multiscale Finite Volume Method.
MSHFEM	-	Multiscale hybrid Finite Element finite Volume Method.
FEA	-	Finite Element Analysis.
PDE	-	Partial Differential Equation.
XFEM	-	Extended Finite Element Method.
GFEM	-	Generalized Finite Element Method.
Hp-FEM	-	Higher Polynomial Refinement Finite Element Method.
DG-FEM	-	Discontinuous Galerkin Finite Element Method.
<i>p</i> -AFEM	-	Polynomial Adaptive Finite Element Method.
te	-	Transition element.
TH	-	Threshold.
CP	-	Corner Point.
e	-	Element.
CM	-	Connection Matrix.
Sol	-	Solver.
LtoG	-	Local to Global.
Flops	-	Floating-point operation per second.
LFEM	-	Linear FEM.
QFEM	-	Quadratic FEM.
RK4	-	Runge-Kutta of order 4.

CR	-	Critical Region.
EB	-	East Boundary.
SB	-	South Boundary.
WB	-	West Boundary.
NB	-	North Boundary.
AEB	-	Adjusted East Boundary.
RK4	-	Runge-Kutta of order 4.
FEV	-	Coupled Finite Element and Finite Volume.
AWB	-	Adjusted West Boundary.
LFE	-	Length of FE.
LFV	-	Length of FV.
NIST	-	National Institute of Standards and Technology.

## LIST OF SYMBOLS

$u$	-	Displacement.
$\Omega$	-	Domain of Interest.
$\Omega_{FE}$	-	The domain of Finite Element Method.
$\Omega_{FV}$	-	The domain of Finite Volume Method.
$K$	-	Stiffness Matrix.
$M$	-	Mass Matrix.
$F$	-	Force vector.
$F^{FEV}$	-	FEV Force vector.
$K_{FE}$	-	FEM expanded Stiffness Matrix.
$K_{FV}$	-	FVM expanded stiffness Matrix.
$K^{AEB}$	-	FEM stiffness Matrix with the adjusted east boundary.
$K^{AWB}$	-	FVM stiffness Matrix with the adjusted west boundary.
$K_{FEV}$	-	Finite Element Volume Stiffness Matrix.
$\kappa(A)$	-	Condition number of Matrix A.
$\ e\ _2^{LFE}$	-	Linear FEM Norm2error.
$\ e\ _2^{QFE}$	-	Quadratic FEM Norm2error.
$\ e\ _2^{MS}$	-	Multiscale FEM Norm2error.
$\ e\ _2^{FV}$	-	Multiscale hybrid FEM Norm2error.
$e_{FE}^L$	-	Linear finite element residual error.
$e_{FE}^Q$	-	Quadratic finite element residual error.
$R^L$	-	Linear FEM residual.
$R^Q$	-	Quadratic FEM residual.
$\Gamma$	-	FEM boundary.
$\Gamma_N$	-	Neumann boundary.
$\Gamma_D$	-	Dirichlet boundary.

$\tau$	-	Diffusion coefficient.
$N_i$	-	<i>ith</i> shape function.
$N_i^L$	-	Linear <i>ith</i> shape function.
$N_i^Q$	-	Quadratic <i>ith</i> shape function.
$nx$	-	Number of Element in the x-direction.
$ny$	-	Number of Element in the y-direction.
$g_n$	-	The gradient at node n.
$nel$	-	The number of elements.
$nno$	-	Number of Nodes.



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# CHAPTER 1

## INTRODUCTION

### 1.1 Motivation

With the rapid advance in computer power, numerical simulations have become a very important method for solving questions in engineering and science. Instead of adopting the traditional theoretical practice using assumptions and approximations to simplify problems, this numerical approach addresses the original problem in all its detail with little assumptions. Providing validation for theories, providing insight into experimental results, and providing help in interpreting or even discovering new phenomena on varied scales, hence, it is a valuable instrument in science (Jebahi *et al.*, 2016; Zeng and Qin, 2018).

A numerical simulation can typically be divided into four scales. The nanoscopic scale, where phenomena related to the behavior of electrons become significant, the microscopic scale, where phenomena related to the behavior of atoms are considered. The mesoscopic scale at which defects in lattices are studied. The macroscopic scale which allows continuum mechanics to explain macroscopic phenomena. Each scale has been addressed by several numerical methods (Weinan and Lu, 2011; Jebahi *et al.*, 2016; Zeng and Qin, 2018).

There are two classes of numerical methods: discrete methods (DM) and continuum methods (CM). Discrete mechanics is the first class and covers the first three scales. They are quantum mechanical methods (QMs) used for nanoscopic analysis, atomistic methods (AMs) used for microscopic analysis, and mesoscopic discrete methods (MDMs) used for mesoscopic analysis. Although the class can provide extremely accurate results, but it is considerably time-consuming and is only suitable for small physical systems (Weinan and Lu, 2011; Jebahi *et al.*, 2016; Zeng and Qin, 2018). Continuous methods (CMs) are based on continuum mechanics and are focused on solving macroscopic problems. Nonetheless, handling additional

episodes of fine scale phenomena is generally necessary. Although continuous methods are less accurate than discrete ones, but they are relatively inexpensive and flexible for large systems (Jebahi *et al.*, 2016; Zeng and Qin, 2018).

Simulations of modern materials have been challenged by multiscale phenomena. Such phenomena require on one scale an extremely accurate and computationally expensive description, and on another scale a coarser description that avoids prohibitively large calculations. Since all DMs and CMs methods alone are not sufficient to describe the entire system, so coupling approaches combining different methods at different scales would be beneficial in distributing computation effort as needed. As a result, multiple multiscale coupling approaches have since been developed to assess mechanical behavior of materials at all relevant scales while retaining accuracy of the individual approaches at each scale (Jebahi *et al.*, 2016; Zeng and Qin, 2018). From all developed multiscale approaches, the concurrent continuum-continm multiscale methods are very few. Most of the concurrent models in the literature are coupling of atomicity and countinnum models (Fish, 2010; Yamashita *et al.*,2016). Thus, the motivation for the adoption of the concurrent continuum-continm multiscale model in this work.

## **1.2 Background of the Problem**

The academic interest in the adoption of multiscale methods for solving physics and engineering problems has been on the increase. This ramped interest had been inspired by factors such as the complex and ‘multiscale’ nature of many application problems across wide spheres of knowledge, the breakthroughs, and rapid appreciations in computing science, and essentially the imperative accuracy and efficiency that highly detailed multiscale and multi-physics problems require. It is usually too exorbitant to compute on the tiniest scale problems that integrate a wide range of scales in the coefficients or solutions. This is without regard to when sophisticated super-computers are deployed. This is largely due to the many unknowns inherent in finest scales, especially if what is of interest are relatively longer lengths and time scales.

Computing on a coarser scale, however, exclusively, may tend towards inaccuracy, as finest scale properties usually seriously impinge on coarse-scale behaviours. Moreover, the case had always been that the coarse-scale properties and guiding equations lack proper definition. It is worthy of note that existing multiscale methods are a hybrid of fine-scale and coarse-scale computational techniques aimed at efficiently resolving the most important fine-scale data without the need for a recourse to direct computation usually associated with global fine-scale problems.

As encapsulated in Car and Parrinello (1985), Zhang *et al.* (1999), and Li and Weinan (2005), the foregoing has application in solid mechanics where the coarse-scale (macroscopic) continuum theory conflates molecular dynamics on the fine-scale (microscopic) to achieve accuracy in the appreciation of macroscopic properties of materials. It also has application in computational fluid dynamics where hydrodynamics and kinetic models, which are respectively on coarse-scale and fine-scale, are integrated to capture the allocation of shocks (Le Tallec and Mallinger, 1997; Schwartzentruher and Boyd, 2006). Multiscale methods equally have application in the critical study of turbulent flow (Pal and Ganesan, 2015) and nano materials (Liu *et al.*, 2004). Flow in porous media is another important application area for multiscale methods.

### **1.3 Statement of the Problem**

Over the years, there have been satisfactory results associated with the adoption of the adaptive finite element method (AFEM) and finite volume method (FVM) is offering a panacea to various kinds of problems that exhibit rapid changes or sharp fronts or wiggles in their numerical solutions (high gradient problems). However, hybridizing the AFEM and finite volume (AFEM/FVM) methods allows the creation of multiscale models that afford the employment of different material models at different levels in different subdomains of the same system. While some parts allow for the adoption of the FV model, AFEM, on the premise of the continuum mechanics model, can be used in other parts. The FVM is ultimately suitable for modelling materials with the tendency for discontinuities and failure,

mostly typified by fracture, shocks, inter alia (Fallah *et al.*, 2000). The AFEM, on the other hand, is usually involved linear and nonlinear continuous material behaviour in solving high gradient problems.

However, this work aims at treating FVM and AFEM as complementary methods in a bid to optimize the advantages of each method. This will have utility in high gradient problems, where numerical errors are inevitable with sudden modifications in numerical solutions. The study is desired to obtain and optimize the hybridized properties of AFEM and FVM. Also, to refine high gradient zones locally to enhance potential solutions' accuracy, thereby developing a numerical model that requires less computational cost and time. The research will ultimately clarify the following questions:

1. How can the advantages of both AFEM and FVM be optimized?
2. How can multiscale hybridization of AFEM and FVM be achieved?
3. How can the solution accuracy in the newly proposed multiscale hybrid method be improved?
4. Where and how can the newly proposed multiscale hybrid technique be applied?
5. How can the speed of the new multiscale hybrid technique be optimized?

#### **1.4 The Study Objectives**

The ultimate objective is to conflate the adaptive finite element method with the finite volume method to afford enhanced solutions to high gradient problems. The following are the main objectives to achieve the goal:

1. To develop an adaptive finite element method (AFEM).
2. To develop a coupled AFEM and finite volume method (FVM).
3. To compare the numerical results of the models with existing analytical solutions.

## **1.5 Scope of the Study**

Several collections of hybrid techniques exist in literature; however, this work focuses on the coupling of  $p$ -adaptive finite element ( $p$ -AFEM) method and finite volume method to produce a multiscale hybrid technique with improved accuracy and efficiency. The formulation and application of the anticipated new technique are restricted to regular high gradient problems in two-dimension. The tools used to compute the numerical results are codes written in OCTAVE and MAPLE programming languages.

## **1.6 Significance of the Study**

In most of the previous studies, the sequential continuum-continuum multiscale models were considered chiefly. This has created a wide gap in the study of the concurrent continuum-continuum models. In order to bridge the gap, this work is based on coupling a concurrent continuum-continuum multiscale model. The coupling of two continuum methods, the Lagrange method (AFEM) and the Eulerian method (FVM), is considered. The work is premised on the accuracy of AFEM and the speed of FVM to develop an improved mathematical model and algorithm. The proposed hybrid technique, envisaged as the research outcome, can produce higher precision results, and require less time for numerical operations. This makes it a veritable technique for solving large domain size and deformations problems. The acquired results equally have practical applications in studying high gradient problems in both engineering and mathematical fields. In addition, the outcomes can stimulate new gaps that can be leveraged upon for further research in related areas.

## **1.7 The Thesis Layout**

The work consist of six chapters and the chapters are structured as follows: The background of the problem is introduced in chapter 1, followed by the problem statement and the study objectives. Also, analysis is done on the study scope and significance. Finally, the layout of the thesis is established.

Chapter 2 provides a comprehensive review of earlier studies on FE technique, FV technique, multiscale techniques, multiscale FE techniques, multiscale FV techniques, hybrid multiscale FE/FV technique, adaptive techniques, Runge-Kutta methods, high gradient boundary value problems, the intricate reasons for coupling and the research gap.

In Chapter 3, the finite element method and the finite volume methods are designed. The validation techniques and robust residual error analysis theorem based on matrix condition numbers are discussed.

Chapter 4 is based on the development of the  $p$ -adaptive finite element method ( $p$ -AFEM), time-dependent FEM,  $p$ -adaptive finite element method error analysis and the numerical validation of the techniques.

In Chapter 5, a proposed numerical technique hinged on the coupling of  $p$ -AFEM and finite volume method is designed. The formulation of error analysis for the new technique is included. The efficiency and feasibility of the proposed new technique are validated with high gradient problems having accessible analytical solutions. The new method is finally applied to two standard high gradient problems and two engineering problems namely the electrostatic and torsion problems.

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

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