COUPLING OF ADAPTIVE REFINEMENT WITH VARIATIONAL MULTISCALE ELEMENT FREE GALERKIN METHOD FOR HIGH GRADIENT PROBLEMS

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Dedicated to my beloved

father, Pooi Chen,
mother, Kam Yin
and my siblings, Siaw Veen,
Yee Loon and Yee Lean
for their endless love, care and support

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ABSTRACT

In this thesis, a new adaptive refinement coupled with variational multiscale element free Galerkin method (EFGM) is developed for solving high gradient problems. The aim of this thesis is to propose a new framework of moving least squares (MLS) approximation with coupling method based on the variational multiscale concept. Additional new nodes will be inserted automatically at high gradient regions by adaptive algorithm based on refinement criteria. An enrichment function is embedded in the MLS approximation for the fine scale part of the problem. Besides, this new technique will be parallelized by using OpenMP which is based on shared memory architecture. The proposed new approach is first applied in two-dimensional large localized gradient problem, transient heat conduction problem as well as Burgers' equation in order to analyze the accuracy of the proposed method and validated with an available analytic solutions. The obtained numerical results show a very good agreement with the analytic solutions and is able to obtain more accurate results than the standard EFGM. It is found that the average relative error of this new method is reduced in the range of 15% to 70%. Besides, this new method is also extended to solve two-dimensional sine-Gordon solitons. The results obtained show good agreement with the published results. Moreover, the parallelization of adaptive variational multiscale EFGM can improve the computational efficiency by reducing the execution time without loss of accuracy. Therefore, the capability and robustness of this new method has the potential to investigate more complicated problems in order to produce higher precision solutions with shorter computational time.

ABSTRAK

Dalam tesis ini, satu kaedah baru berdasarkan gabungan penyesuaian penghalusan dengan kaedah multiskala ubahan tanpa unsur Galerkin (EFGM) telah dibangunkan untuk menyelesaikan masalah dengan kadar perubahan tinggi. Matlamat tesis ini adalah untuk mencadangkan satu rangka kerja baru penghampiran jenis pergerakan kuasa dua terkecil (MLS) dalam kaedah gabungan ini berdasarkan konsep multiskala ubahan. Algoritma penyesuaian akan memasukkan nod tambahan baru secara automatik di kawasan kecerunan tinggi berdasarkan kriteria penghalusan. Suatu fungsi tambahan akan digunakan dalam anggaran jenis MLS dalam bahagian skala halus pada masalah tersebut. Selain itu, teknik baru pengiraan ini akan diselarikan dengan menggunakan OpenMP yang berasaskan seni bina perkongsian memori. Kaedah cadangan baru ini akan digunakan untuk menyelesaikan masalah dua dimensi kecerunan tinggi setempat, masalah pengaliran haba serta persamaan Burgers untuk menganalisis ketepatan kaedah ini dan disahkan dengan penyelesaian sebenar. Keputusan berangka yang diperolehi menunjukkan penyesuaian yang sangat baik dengan penyelesaian analitik dan mampu memperolehi keputusan yang lebih tepat berbanding dengan EFGM piawai. Didapati bahawa purata ralat relatif kaedah baru ini boleh dikurangkan dalam lingkungan 15% hingga 70%. Selain itu, kaedah baru ini juga dikembangkan untuk menyelesaikan dua dimensi soliton sinus-Gordon. Keputusan yang diperolehi menunjukkan penyesuaian yang baik berbanding dengan keputusan yang telah diterbitkan. Tambahan pula, kecekapan pengiraan daripada keselarian penyesuaian multiskala ubahan EFGM boleh dipertingkatkan dengan mengurangkan masa kiraan tanpa kehilangan ketepatan. Oleh sebab itu, keupayaan dan keteguhan kaedah baru ini mempunyai potensi untuk mengkaji masalah yang lebih kompleks untuk menghasilkan penyelesaian yang lebih tepat dengan masa pengiraan yang lebih pendek.

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LIST OF SYMBOLS

$\mathbf{a}(\mathbf{x})$	-	Vector of Unknowns
β	-	Dissipative Term
c_I	-	Size of Compact Support of Node *I* in One-dimensional
cx_I	-	Size of Compact Support in *x* axis of Node *I* in Two-dimensional
cy_I	-	Size of Compact Support in *y* axis of Node *I* in Two-dimensional
d_I	-	Basic Support of Node *I* in One-dimensional
dm	-	Dimensionless Size of the Influence Domain
dx_I	-	Basic Support in *x* Direction of Node *I* in Two-dimensional
dy_I	-	Basic Support in *y* Direction of Node *I* in Two-dimensional
G	-	Differential Operator
$\mathbf{G}(\mathbf{x}_k)$	-	Integrand Value at Gauss Point $\mathbf{x}_k$
G_m	-	Gradient of Node *m*
h_x	-	Spacing of Nodes in *x* Direction
h_y	-	Spacing of Nodes in *y* Direction
h	-	Distance Between Two Particles
$\mathbf{J}_{kj}$	-	Jacobian Associated with Each Gauss Point
m	-	Number of Basis Functions
n	-	Time Level
N	-	Number of Nodes
n_c	-	Number of Background Cells
n_g	-	Number of Gauss Points in Each Background Cell
$\mathbf{n}$	-	Unit Normal to the Natural Boundary
$N_I(s)$	-	Lagrange Interpolation

$\mathbf{p}(\mathbf{x})$	-	Complete Polynomial Basis
$\overline{P}$	-	Linear Projector onto $\overline{V}$
$Q(x, y, t)$	-	Heat Generation Rate
q	-	Dimensionless User-defined Threshold Value
R_I	-	Radius of the Domain Support of Node I
R_0	-	Radius of Domain of Influence for the Original Nodes
R_1	-	Radius of Domain of Influence for the New Nodes
Re	-	Reynold Number
$R(\mathbf{x})$	-	Residual Error
r	-	Normalized Radius
S_p	-	Speedup
T	-	Temperature Distribution
T_1	-	Execution Time Spend on One Processor
T_p	-	Execution Time Spend on p Processor
$\bar{t}$	-	Prescribed Traction on Natural Boundary
t	-	Time Level
$u^h(\mathbf{x})$	-	Moving Least Squares Approximation Function
u_E	-	Prescribed Displacement on Essential Boundary
u	-	Velocity u
$\overline{u}^h(\mathbf{x})$	-	Coarse Scale Approximation
$\hat{u}^h(\mathbf{x})$	-	Fine Scale Approximation
v	-	Velocity v
$\overline{V}$	-	Coarse Scale Subspace
$\hat{V}$	-	Fine Scale Subspace
w_k	-	Gauss Weighting Factor for the k^{th} Gauss Point
$w_I(\mathbf{x})$	-	Weight Function
$\overline{w}$	-	Weighting Function in Coarse Scale
$\hat{w}$	-	Weighting Function in Fine Scale
Ω	-	Domain of Interest
$\phi_I(\mathbf{x})$	-	Moving Least Squares Shape Function

$\boldsymbol{\Psi}$	-	Test Function
λ	-	Lagrange Multipliers
α	-	Penalty Parameter
$\overline{\phi}$	-	Coarse Scale Shape Function
$\hat{\phi}$	-	Fine Scale Shape Function
Γ_u	-	Essential Boundary
Γ_t	-	Natural Boundary
δ_{IJ}	-	Kronecker Delta Function
Δt	-	Time Step

LIST OF ABBREVIATIONS

DEM	-	Diffuse Element Method
DOI	-	Domain of Influence
EFG	-	Element Free Galerkin
EFGM	-	Element Free Galerkin Method
FDM	-	Finite Difference Method
FEM	-	Finite Element Method
FE	-	Finite Element
Flop	-	Floating point operation
Flops	-	Floating point operations per second
GB	-	Gigabyte
GHz	-	Gigahertz
HAM	-	Homotopy Analysis Method
LBIE	-	Local Boundary Integral Equation
MLS	-	Moving Least Squares
MLPG	-	Meshless Local Petrov-Galerkin
MPI	-	Message Passing Interface
ODE	-	Ordinary Differential Equation
OpenMP	-	Open Multi-Processing
PDE	-	Partial Differential Equation
PVM	-	Parallel Virtual Machine
RAM	-	Random Access Memory
RKPM	-	Reproducing Kernel Particle Method
SPH	-	Smoothed Particle Hydrodynamics

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CHAPTER 1

INTRODUCTION

1.1 Introduction

In this chapter, the background of the problem will be briefly introduced. After that, statement of the problem and objectives of the study will be clearly defined. Besides, the scope of the study will be discussed as well as the significance of the study. Lastly, for clarity, the layout of the thesis is briefly outlined.

1.2 Background of the Problem

The finite element method (FEM) has been widely used by researchers to approximate the solution of partial differential equations. However, the FEM has its drawbacks as this is a mesh-based method and highly reliance on meshes. When dealing with large deformation or high gradient problems, the FEM will produce lower accuracy solutions due to the mesh become extremely skewed or compressed. Moreover, the FEM is also not well suited for discontinuous solutions since the element edges must be aligned to the discontinuity. To overcome these difficulties, the re-meshing process is needed to avoid mesh distortion and allows mesh line to remain coincident with any discontinuities. However, this re-meshing process is tedious and leads to degradation in computational efficiency. Thus, the FEM is not an ideal method to couple with adaptive refinement as the re-meshing of the problem domain is necessary in every computational time step.

The meshfree methods [1,2,3,4,5,6,7,8,9] have been proposed as an alternative numerical techniques to the FEM. This class of numerical methods solve the problem through constructing the function based on a series of scattered points over the problem domain. Although the re-meshing process can be avoided in the meshfree methods, but this advantage does not come cheap. In particular, the computational cost in element free Galerkin method (EFGM) is much more expensive than the FEM. The increased in computational cost is especially evident for adaptive refinement analysis due to the computation of moving least squares (MLS) shape functions which are formulated at every integration point. The high computational cost is the predominant drawback of EFGM. Furthermore, the EFGM also encounters difficulty in enforcing the essential boundary conditions as its shape functions do not satisfy the Kronecker delta property. Therefore, several methods have been proposed to overcome this problem, in particular, Lagrange multiplier method [1], penalty method [10] and coupling to finite element method [11]. However, the drawback of Lagrange multiplier method is additional unknowns are introduced. In contrast, coupling to finite element method requires well-defined boundary meshes.

The EFGM is an ideal technique to solve steep gradient or rapid variations problems due to the property of meshfree approximations with no nodal connectivity is needed. However, special care must be taken to capture the solution precisely near the high gradient regions and to avoid numerical pollution. A number of techniques have been used in dealing with high gradient problems. The first technique is to refine the spatial discretization near the locally high gradient computation region as reported in References [12,13,14]. In these papers, dense of nodes are moved with the crack tip at each step to provide a more accurate solution. Besides, a higher order quadrature will be used in all the cells where the crack would possibly occur [15,16,17], but this technique will increase the computational cost. Another approach is to use an enriched basis as conducted in [18,19]. However, the enrichment of the trial functions proposed in [19] introduces additional unknowns and considerable computer programming is required. Therefore, more research efforts should be devoted by researchers for solving problems involving sharp gradient or rapid variation in solutions.

1.3 Statement of the Problem

Adaptive EFGM and variational multiscale EFGM have been numerous reported to solve various kind of problems with satisfactory results obtained. In dealing with sharp gradient problems, numerical errors may occur due to the abrupt change in numerical solutions. Hence, it is desired to obtain the good properties of adaptive EFGM and variational multiscale EFGM to refine the high gradient zones locally in order to get more accurate solutions. Therefore, the development of a numerical model with combination of both properties with less computational cost is in demand. This is the intention of this thesis and this research will clarify the following questions:

1) How to overcome the deficiency in penalty method for EFGM?

2) How to obtain good properties of adaptive EFGM and variational multiscale EFGM?

3) How to improve the solution accuracy in the proposed new method?

4) What is the application of the proposed new technique?

5) How to reduce the execution time in numerical analysis of the proposed new scheme?

1.4 Objectives of the Study

The principal goal of this thesis is to couple the adaptive refinement analysis with variational multiscale EFGM for high gradient problems. The five main objectives associated with the principal goal are as follows:

1) To improve the penalty method for EFGM and apply it to enforce the essential boundary conditions.

2) To couple the adaptive EFGM with variational multiscale EFGM and develop its numerical solution procedure.

3) To propose a new moving least squares approximation function to improve the solution accuracy by enhancing the shape functions with an enrichment function.

4) To apply the proposed new technique to high gradient problems as well as sine-Gordon solitons.

5) To develop and implement a parallel computer code using Open Multi-Processing (OpenMP) application programming interface in the proposed new scheme.

1.5 Scope of the Study

There are many sets of meshfree methods available in literature. This research will only focus on one of the meshfree methods, in particular element free Galerkin method. Moreover, the development and implementation of the proposed new scheme is limited to two-dimensional regular high gradient problems. The computational tool used to compute the numerical result is C programming language. Furthermore, the parallel programming scheme developed in this work is focused on OpenMP which is based on share memory architecture.

1.6 Significance of the Study

The methods for imposition of essential boundary conditions are the essential tool for EFGM. In this work, the penalty method used in EFGM has been improved and higher accuracy results are obtained compared with the classical penalty method. The mathematical model and algorithm produced in this work will combine the good properties of adaptive refinement analysis and variational multiscale EFGM. In addition, the proposed coupling method with parallelization is capable to produce higher precision results with less time consumption. Thus, this technique is ideally used to solve large deformations problems as well as large domain size problems. The obtained results will be beneficial in the study of large gradient problems in mathematics and engineering fields. Also, the findings obtained can be used for further research in related areas.

1.7 Layout of the Thesis

This thesis consists of seven chapters and it organized as follows:

Chapter 1 starts with the background of the problem, statement of the problem and objectives of the study. In addition, the scope and significance of the study are also demonstrated.

Chapter 2 presents a detailed literature review of previous studies on meshfree methods, element free Galerkin method, variational multiscale meshfree methods, adaptive meshfree methods, parallel computing, OpenMP and sine-Gordon equation.

In Chapter 3, the standard penalty method has been improved for enforcing essential boundary conditions in EFGM. This chapter starts with the development of the moving least squares approximation. The fundamentals required for the numerical implementation in EFGM are reviewed such as efficient calculation of MLS shape functions and derivatives, determination of domain of influence and the weight function. A discussion on Lagrange multiplier method and penalty method used for enforcing essential boundary conditions in EFGM are given. Also, an improved penalty method is introduced to impose the essential boundary conditions and validated with a numerical problem with Dirichlet and mixed boundary conditions.

In Chapter 4, a new approach based on the coupling of adaptive EFGM and variational multiscale EFGM is developed. A discussion on adaptive procedures such as the refinement criteria, refinement strategy and data mapping are provided as well as the description on variational multiscale method. Additionally, the formulation of a new MLS approximation is described in detail. The description on the coarse scale shape functions and the fine scale shape functions with enrichment function are also outlined. An efficient computation of fine scale shape functions and its derivatives are also considered. Furthermore, a numerical solution procedure based on the combination of refinement procedure and variational multiscale procedure is introduced. The formulation of error analysis for the new approach is shown. The feasibility and efficiency of the proposed new scheme are validated with three high gradient problems with available analytical solutions.

Chapter 5 extends the new scheme presented in Chapter 4 to solve two-dimensional sine-Gordon solitons. The problem description of two-dimensional sine-Gordon equation is illustrated. The formulation of adaptive variational multiscale EFGM for sine-Gordon equation is demonstrated. Two two-dimensional sine-Gordon solitons problems are examined to verify the performance of the proposed new scheme and the solutions obtained are validated with results from the literature.

In Chapter 6, a shared memory parallel computer implementation is developed. The parallel execution scheme in OpenMP and the performance of parallel programs are illustrated. In addition, the implementation of parallel scheme in the new coupling approach is given. The performance of the parallel implementation is validated with solving two numerical problems and analyzed with the corresponding serial implementation.

Finally, conclusions are drawn and recommendations for future research are illustrated in Chapter 7.

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