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A Computational Framework for the Development of a Stochastic Micro-Cracks Informed Damage Model

A dissertation submitted in partial satisfaction of the requirements for the degree Doctor of Philosophy in Civil Engineering

by

Shih-Po Lin

2014
ABSTRACT OF THE DISSERTATION

A Computational Framework for the Development of a Stochastic Micro-Cracks Informed Damage Model

by

Shih-Po Lin

Doctor of Philosophy in Civil Engineering

University of California, Los Angeles, 2014

Professor Jiun-Shyan Chen, Chair

The objective of this research is to develop the multi-scale mathematical formulation and the associated numerical techniques for development of a micro-crack informed stochastic damage model for brittle materials with application to fragment-impact modeling of concrete materials.

A Generalized Stochastic Chaos (GSC) method has been developed in this work. In this approach, the radial basis (RB) and reproducing kernel (RK) approximations have been introduced to represent the stochastic process which provide flexibility in adjusting smoothness and locality in the finite dimensional stochastic spaces. In conjunction with the RK and RB approximations, a collocation method has been employed for solving the
stochastic partial differential equation. In this manner, the stochastic system is discretized into a set of deterministic systems that can be solved separately, and the approximation can be tailored according to the characteristics of the stochastic systems under consideration.

The GSC method has been applied to the development of stochastic damage law based on homogenization of microstructures with random voids. In this development, an extrinsic enrichment method under the framework of mesh-free methods has been introduced for modeling micro crack propagation in the RVE. The near-tip field is discretized by utilizing the visibility criterion in conjunction with crack-tip enrichment while preserving the Partition of Unity (POU) property, which guarantees the conservation of mass. Furthermore, an integration method which meets the so called integration constraint has been proposed to enhance the solution accuracy near the crack tip without using the inefficient higher order Gauss quadrature rules.

In the homogenization processes, the characteristics of the stochastic representative volume element (SRVE) have been investigated. The existence of SRVE has been confirmed through the satisfaction of the Hill condition, ergodicity and the principle of the minimum potential energy. The size effect and mesh dependency of the damage model are also demonstrated by using the principle of the minimum potential energy. The mesh dependency issue has been resolved by introducing a length-scale into the homogenized damage evolution equation. Finally, a two-parameter multi-scale damage model has been developed under the

iii
framework of the SRVE. The proposed model is then validated through the comparison between numerical simulations and experimental observations of an ultra-high strength concrete subjected to trial axial compression with various levels of confinement.
The dissertation of Shih-Po Lin is approved.

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CONTENTS

CHAPTER 1. Introduction ................................................................. 1

1.1 Motivation ............................................................................. 1
1.2 Objective and Scope ............................................................... 2

CHAPTER 2. Literature Review ...................................................... 5

2.1 Overview of Stochastic Theories .............................................. 5
2.2 Overview of Galerkin and Collocation Reproducing Kernel Methods ................................................................. 8
2.3 Overview for the Modeling of Crack Propagation .................... 10
2.4 Overview of Multi-scale Methods ............................................ 13

CHAPTER 3. Basic Equations in Stochastic Methods ...................... 16

3.1 Stochastic Boundary Value Problems ...................................... 16
3.2 The Karhunen-Loève Expansion ............................................. 16
3.3 The Monte Carlo Simulation .................................................. 20
3.4 The Neumann Expansion ...................................................... 21
3.5 Stochastic Galerkin and Collocation Methods ......................... 23
3.6 The Homogeneous Chaos ..................................................... 27
3.7 Selection of Collocation Points by using the Smolyak Algorithm ... 30

CHAPTER 4. The Generalized Stochastic Chaos (GSC) .................. 37

4.1 The Reproducing Kernel (RK) Approximation ......................... 37
4.2 The Radial Basis Function (RBF) Approximation .................... 41
4.3 Accelerated RK and RB Approximations in the Random Space ….. 42
4.3.1 Accelerated RK Approximation in the Uniform Domain …….. 43
4.3.2 Computational Reduction for Multi-dimensional Problems … 44
4.4 Numerical Examples for Solving Stochastic Boundary Value Problems ……………………………………………………. 50
4.4.1 The RK and RBF Approximations for Smooth Functions ….. 50
4.4.2 The Kraichnan-Orszag Three-mode Problem ………………. 53
4.4.3 A Cantilever Subjected to a Uniform Distributed Load …….. 56

CHAPTER 5. Crack Modeling Using Enriched RKPM 58
5.1 Formulation of Extrinsically Enriched RKPM ……………….. 58
5.2 An Explicit Time Integration Method for Crack Propagation ….. 63
5.2.1 A Lumped Mass Scheme ……………………………………… 63
5.2.2 Update of the Nodal Coefficients of Additional Bases due to Crack Propagation ……………………………………… 64
5.3 A High Order Stabilized Conforming Nodal Integration for Galerkin Meshfree Approximation ……………………………… 67
5.4 Numerical Verification of Bench Mark Problems …………….. 74
5.4.1 Stationary and Moving Mode I Crack Problems …………….. 74
5.4.2 An Edge-cracked Plate under Impulsive Loading ………….. 76
5.4.3 Convergence Study of Motz's Problem …………………….. 78
5.4.4 A Stationary Edge-crack Problem ……………………. ……. 80
5.4.5 A Three-point Bending Specimen with Cohesive Zone Modeling ……………………………………………………. 83
5.4.6 A Single Edge Notched Beam …………………………. 84
CHAPTER 6. The Stochastic Multi-scale Modeling

6.1 The Characteristics of the Stochastic Representative Volume Element .............................................................. 86

6.2 Size Effect of the Micro-crack Informed Multi-scale Damage model ................................................................. 103

6.3 A Remedy for Size Effect ......................................................... 112

6.4 A Two-parameter Damage Model ........................................... 117

6.5 Summary ............................................................................. 122

CHAPTER 7. Applications

7.1 The Characteristics of the Concerned Brittle Material ............... 124

7.2 Hierarchies of the Material Moduli ......................................... 126

7.3 Tri-axial Compression Tests of the Ultra-high Strength Concrete with the Stochastic Multi-scale modeling ............. 129

CHAPTER 8. Conclusions and Future Work

8.1 Summary of Developments .................................................... 140

8.2 Suggestions for Future Work ............................................... 143

REFERENCES

viii
LIST OF FIGURES

Figure 3.1 The plots of exponential covariance function ............................ 19
Figure 3.2 Different levels of discretization for 1-D approximation scheme ... 34
Figure 3.3 The nodal sets for the combination of 1-D approximation schemes with different levels ........................................ 35
Figure 3.4 The number of the required nodes for Somlyak algorithm up to order q and the full set as ........................................... 36
Figure 4.1 (a) The RK discretization and compact support in two-dimension (b) the RK basis function ................................................. 40
Figure 4.2 Equal-interval discretization for the RK approximation scheme ... 44
Figure 4.3 Equal-interval discretization with extra virtual nodes for the RK approximation scheme ........................................... 44
Figure 4.4 Comparison of L2 error norm between two different schemes ..... 51
Figure 4.5 Error norm vs. number of nodes ........................................... 52
Figure 4.6 The layout of the nodes as N=6 ........................................... 52
Figure 4.7 Comparisons among different approximation schemes .......... 55
Figure 4.8 A cantilever beam subjected to a uniform distributed load ........ 56
Figure 4.9 The comparison for the average and standard deviation of the beam tip deflection among different numerical methods ............. 57
Figure 5.1 A crack in a domain with the mesh-free approximation .......... 59
Figure 5.2 The graphical illustration for the heaviside enrichment function .. 61
Figure 5.3 The illustration of crack tip enrichment functions ................. 62
Figure 5.4 The changing discretization near the crack tip field .......... 65
Figure 5.5  A body with a crack involving a cohesive zone ................. 68
Figure 5.6  Geometrical definition of a nodal domain ...................... 71
Figure 5.7  Semi-infinite crack in an infinite plate subjected to a tensile stress wave ................................................................. 75
Figure 5.8  Comparison of the stress intensity factor $K_1$ ..................... 76
Figure 5.9  The schematic description of the edge-cracked plate under impulsive loading ................................................................. 77
Figure 5.10  The final crack path for the edge-cracked plate .................. 77
Figure 5.11  The boundary conditions of Motz's Problem ..................... 78
Figure 5.12  Comparisons for L2 error norms among different integration methods ................................................................. 80
Figure 5.13  Comparisons for Semi-H1 error norms among different integration methods ................................................................. 80
Figure 5.14  A plate with an edge crack ............................................ 81
Figure 5.15  Comparisons of $K_1$ under different integration schemes ......... 82
Figure 5.16  A three-point bending beam .......................................... 83
Figure 5.17  Load-deflection curves of a 3-point bending problem .......... 84
Figure 5.18  A single edge notched beam .......................................... 85
Figure 5.19  Load-COD curves of the mixed mode fracture problem ......... 85
Figure 6.1  A 2-D sinusoidal of function with infinite domain ............... 90
Figure 6.2  Partitions of a microscopic cell in domain $\Omega$ ..................... 93
Figure 6.3  Illustration for meso-scale bounds of material moduli .......... 101
Figure 6.4  Standard deviation vs. RVE size .................................... 102
Figure 6.5  Microscopic and macroscopic structures .......................... 104
Figure 6.6  Homogenization of a microscopic cell  ......................... 104
Figure 6.7  Periodic micro-structure with micro-cracks  ...................... 110
Figure 6.8  Illustration of the size effect of periodic micro-structures  ....... 111
Figure 6.9  Size effect of model refinement  .................................. 111
Figure 6.10  Size effect of stress and strain curves  ............................ 112
Figure 6.11  Samples of different microscopic cell sizes  ....................... 112
Figure 6.12  Average homogenized stress-strain curves of different RVE sizes ................................. 113
Figure 6.13  Average homogenized damage evolution curves of different RVE sizes ......................................................... 113
Figure 6.14  A notched beam subjected to three-point bending ............... 114
Figure 6.15  The size effect curve of nominal strength  ........................ 114
Figure 6.16  Mesh dependent load–displacement responses using inconsistent sizes of the microscopic cells ................................. 116
Figure 6.17  Average approximated and homogenized damage evolution curves of different RVE sizes ................................. 116
Figure 6.18  Mesh independent load–displacement responses using the damage evolution function with a scaling law ............................. 116
Figure 6.19  Different loading cases for microscopic cell analyses ............ 119
Figure 6.20  Modified yield surface of AFC model  ............................. 121
Figure 7.1  The procedures of the multi-scale modeling  ......................... 124
Figure 7.2  Sampled CT scans of a ultra-high strength concrete ............... 125
Figure 7.3  Construction of numerical model through image segmentation .... 125
Figure 7.4  Samples of different microscopic cell sizes  ......................... 127
Figure 7.5  Convergence of the material moduli w. r. t. various RVE sizes …… 128
Figure 7.6  Standard deviation of the material moduli w. r. t. various unit cell sizes ……………………………………………………………………… 128
Figure 7.7  Approximation of PDF by using Kernel Density Estimation ……. 130
Figure 7.8  RVE analyses under pure shear boundary condition …………… 133
Figure 7.9  RVE analyses under uni-axial boundary condition ……………… 134
Figure 7.10 Failure patterns of an RVE sample under different loading Conditions …………………………………………………………… 134
Figure 7.11 Peak stress-porosity curves ……………………………………… 134
Figure 7.12 Comparisons of the tri-axial compression tests ………………… 138
## LIST OF TABLES

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Table 3.1</td>
<td>One dimensional polynomial chaos</td>
<td>29</td>
</tr>
<tr>
<td>Table 3.2</td>
<td>Two dimensional polynomial chaos</td>
<td>30</td>
</tr>
<tr>
<td>Table 4.1</td>
<td>Operation counts for solving full matrices (global approximation)</td>
<td>48</td>
</tr>
<tr>
<td>Table 4.2</td>
<td>Operation counts for solving banded matrices (local approximation)</td>
<td>50</td>
</tr>
<tr>
<td>Table 4.3</td>
<td>CPU time for solving generalized coefficients</td>
<td>51</td>
</tr>
<tr>
<td>Table 5.1</td>
<td>Comparison of error in K1 (%) using RKPM with higher order SCNI and XFEM</td>
<td>82</td>
</tr>
<tr>
<td>Table 7.1</td>
<td>Particle distribution analysis</td>
<td>125</td>
</tr>
<tr>
<td>Table 7.2</td>
<td>Normalized STDs of the homogenized material properties</td>
<td>135</td>
</tr>
<tr>
<td>Table 7.3</td>
<td>Parameters of the modified AFC model</td>
<td>136</td>
</tr>
</tbody>
</table>
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Publications & Presentations


Chapter 1

Introduction

1.1 Motivation

In reality, uncertainties exist in all natural phenomena, where the randomness is resulting from the “nature of irregularity”. The randomness can be reduced by maximizing the observations so as to minimize the uncertainty. In structure analysis for example, the heterogeneity of materials and the irregularity of external excitations exhibit noticeable uncertainties in many applications. Through stochastic processes, the nature of uncertainties and the randomness of the structural behaviors in response to the said uncertainties can be defined. To predict the uncertainties of structural behaviors with numerical analyses, methods considering a large number of simulations have been introduced, such as the Monte Carlo Simulation. Under such approach, a stochastic system requires much demanding computation than a deterministic system, as it requires sampling many possibilities. This calls for an urgent need in the development of effective stochastic computational methods.

In the field of mechanics and materials, the classical continuum mechanics ignores the statistical variations in the microstructural heterogeneous material properties and microstructure geometry. How the statistical variations in the microscale propagate to the continuum scale is yet to be investigated in the field of structural mechanics. Many
microstructural events, such as grain structure evolution in polycrystalline materials, development of micro cracks and nucleations, and evolution of dislocations affect the inelastic behavior of continua such as plastic deformation, strain localization, shear banding, fatigue, creep, and damage. The randomness in these microstructural events is responsible for the stochastic nature of defects in the materials. This work aims to develop the mathematical formulation and computational framework for investigation of how stochastic microstructural properties such as materials properties, geometries, and micro-cracks affect the stochastic defect properties in the form of continuum damage mechanics.

1.2 Objective and Scope

The objective of this research is to develop the multiscale mathematical formulation and the associated numerical techniques for development of a micro-crack informed stochastic damage model of brittle materials with application to fragment-impact modeling of concrete materials. The main tasks of this research are summarized below:

(1) Development of a generalized stochastic chaos method for representation of the random variables.

Global polynomial based stochastic chaos has been commonly used to represent the random variables. Polynomial chaos formulation is based on the construction of the orthogonal bases with respect to the probability density function. However, the polynomial chaos has been shown to have slow convergence or even fail to converge due to the employment of truncated probability density function in the practical applications. In this work, a generalized stochastic chaos method has been developed to represent the random variables, in conjunction with the collocation method, to overcome the said difficulties.
(2) Development of numerical algorithms for solving stochastic PDEs based on the proposed random variable approximations.

The main challenge in the solution of stochastic PDE is the high computational cost due to the high dimensionality in stochastic space. Such a difficulty is termed as “curse of dimensionality”. By introducing the proposed generalized stochastic chaos approximation, we have developed the associated numerical algorithms for solving stochastic PDEs. The proposed method is based on the framework of collocation method for the sampling of PDE solution in the random space. This includes the enhanced domain integration methods for modeling microcrack propagation in the microstructures, where the near-tip singularity in the strain and stress fields requires sophisticated domain integration techniques for desired accuracy.

(3) Development of stochastic multiscale homogenization for composite microstructures.

The multi-scale method has been well developed for homogenization of deterministic microstructures. The statistical variations of the microstructures, on the other hand, dictate the randomness of the homogenized material properties and behavior. The proposed numerical formulation for stochastic PDEs has been applied to the multiscale homogenization of microstructures. Specific attention has been devoted to the homogenization of two-phase composite materials containing elliptic inclusion with randomness in dimension, orientation, and position.

(4) Development of micro-crack informed stochastic damage model for brittle materials.

The issue of characteristic length scale in the proposed stochastic damage model has been investigated under the homogenization of the stochastic representative volume element (SRVE). The existence of SRVE has been validated through the satisfaction of the Hill condition, ergodicity and the principle of the minimum potential energy. Under this framework, a two-parameter continuum damage model with consideration of the
statistical variations of micro-voids and the associated crack evolution has been developed based on the Helmholtz free energy equivalence between cracked microstructure and homogenized continuum. The proposed micro-crack informed stochastic damage model has been applied to the modeling of the ultra-high strength concrete structures.

The layout of the proposal is organized as follows. In Chapter 2, detailed literature review of the related subjects is provided. Formulation of conventional stochastic theories is given in Chapter 3. In Chapter 4, a generalized stochastic chaos based on Reproducing Kernel approximation and Radial Basis function is introduced and the associated numerical algorithms are proposed to enhance the efficiency of the presented stochastic chaos. The numerical fracture modeling is presented in Chapter 5. The multi-scale formulation based on energy bridging methods and the characteristic length scale analysis will be provided in Chapter 6. Numerical verification and validation will be performed in Chapter 7. Lastly, in Chapter 8 conclusions and the future plan will be outlined.
Chapter 2

Literature Review

2.1 Overview of Stochastic Theories

Due to the fast growth of computer technology, numerical simulations have become an important tool to predict behaviors of complex physical or engineering systems. In reality, the engineering problems possess noticeable uncertainties due to the limitation of knowledge where it is impossible to exactly describe the existing state, a future outcome, or even more than one possible outcome. Uncertainty can be described in several ways, depending on how much information is available. In this dissertation, we focus on boundary value problems with a probabilistic description of the uncertainty in the input data. In the literature, mathematical models have been proposed for solving the stochastic boundary value problems. Babuška et al. [1-2] provided some mathematical concepts for stochastic elliptical partial differential equations. They provided a priori error estimates for the computation of the expected value of the solution under the frameworks of stochastic collocation methods and Galerkin methods. Conventional approaches for solving boundary value problems with random inputs can be divided into two categories: Non-sampling methods and sampling methods.

In the class of non-sampling methods, no repetitive deterministic solvers are employed. Some methods have been proposed for stochastic analysis, such as Neumann Expansion. If the inverse of a given operator exists, the solution can be expanded as a convergent series in
terms of the iterated kernels [3]. This theory was first developed by Neumann and was later investigated by Fredholm [4]. Adomian and Malakian [5] further generalized this inverse method to stochastic partial differential equations and studied its convergence. Yamazaki and Shinozuka [6] as well as Ghanem and Spano [7] developed the Neumann expansion method for evaluating the effect of spatially varying material properties in the linear static structural analysis. Basic statistical properties, such as the mean and the covariance of the solution process, can be effectively determined with this method. Another approach under the category of non-sampling methods is perturbation methods [8-10]. Liu et al. [8-9] proposed a method called probabilistic finite element. The statistical moments up to second order can be obtained by conducting the first order Taylor expansion for the stochastic linear system. However, the perturbation methods are only suitable for problems of random inputs with small deviation. For random inputs with large deviation, the truncated higher order terms of the Taylor series may be so large that they affect the statistical moments. Although one can adopt higher order terms in the Taylor series, the computational cost will be intensively increased and the methods will lose their advantages in terms of computational efficiency over the other methods.

On the other hand, for the sampling methods, the most classical one is the Monte Carlo method, which was first presented by Stanislaw Ulam in 1946, and later named by Von Neumann [11]. The method has been widely used in stochastic analysis to estimate the randomness and uncertainty for many physical and mathematical systems. It can be applied to physical sciences, engineering, statistics, finance and business, games, among others. For structural mechanics, the Monte Carlo simulation (MCS) is an effective way to estimate the randomness and uncertainty of structural systems. The method requires simulation of a sufficient amount of cases corresponding to the random quantities of the physical system and
then processing the simulated results to obtain the statistical properties of the system. Such approach is simple, but computationally expensive due to its slow convergence. For a large sample size $N$, this method offers $1/\sqrt{N}$ convergence for the mean value, as the probability distribution is uniform [12]. For obtaining reliable information from stochastic analysis, sufficient simulations are required. Several sampling schemes are proposed to improve the efficiency of the solution process, for example, the Latin hypercube sampling [13-14] and the quasi Monte Carlo sampling [15-16].

In 1938, Wiener first introduced the so-called “Homogeneous Chaos” method [17], a method for representing an unknown random variable by projecting the solution into a series of Hermite polynomial functionals of a Gaussian process. The functionals are constructed as a Taylor series type with orthogonal properties. The method is considered to be under the category of sampling methods, since the coefficients of the polynomials are determined through Galerkin method, where the quadrature points are treated as special sampling points. For Gaussian processes, the method can achieve an optimal convergence rate, since the weighting function of Hermite polynomials is the same as the probability density function of the random variables of Gaussian processes. It has been proved that the convergence rate of the approximation is exponential [18]. In the finite element analysis, Ghanem and Spanos [19] applied the Homogeneous Chaos method to model the uncertainty in various problems in solid mechanics. Cameron and Martin [20] demonstrated that any functional in $L_2$ approximated with Hermite polynomials can converge in the $L_2$ sense. However, this method is only suitable for Gaussian processes. It can be understood that the weighting function of Hermite polynomials is the same as the probability density function of the Gaussian random variables, so the scheme should be optimal for Gaussian processes. For other types of processes, the convergence rate is slow since the probability density functions of these
processes are not in accordance with the weighting function of the Hermite polynomials.

Xiu and Karniadakis [21] proposed the “generalized polynomial chaos (gPC)” or the “Askey-chaos”, which can be regarded as the generalization of the “Homogeneous Chaos” proposed by Wiener. Here the polynomials are chosen from the hyper-geometric polynomials of the Askey scheme [22]. The bases of the approximation are not restricted to Gaussian processes. They can be other types of random variables without losing the orthogonal properties. The authors further investigated the convergence properties of different bases and proved the convergence rate is exponential for model problems. This method was later applied to steady state diffusion problems [23] and flow simulation [24]. In the standpoint of stochastic analysis, global polynomial based functions are not always good choices for constructing the approximation, since its convergence depends on increasing the order of the basis function. For non-smooth functions, increasing the order of polynomials yields the Gibbs phenomenon. For problems with strong discontinuity, the global polynomial-based approximation schemes converge slowly or even fail to converge [25-26]. In this dissertation, the Reproducing Kernel (RK) function and the Radial Basis Function (RBF) are adopted as the approximation methods in the random space.

2.2 Overview of Galerkin and Collocation Reproducing Kernel Methods

Liu et al. [27] introduced a Reproducing Kernel Particle Method (RKPM) based on a RK approximation as a correction to kernel approximation in the smoothed particle hydrodynamics (SPH). With the correction of the kernel approximation, the continuous reproducing kernel approximation has been constructed to satisfy the polynomial reproducing
conditions. Later, Chen et al. [28] demonstrated that such an approximation can reproduce arbitrary basis functions in a discrete form and incorporated this method to analyze large deformation nonlinear structures. Han and Meng [29] provided a theoretical analysis on the convergence of RKPM. Hu and Chen et al. [30] further studied the error estimation of the RK approximation for the strong form collocation methods, where the RK basis functions with higher smoothness than the finite element interpolation has been utilized. This approach avoids domain integration and thus disposes of the need for generating integration meshes. In these earlier works, the RK approximation offers a better accuracy than the conventional finite element approximation with the same polynomial bases due to its higher order continuity. However, the computational cost for calculating the basis functions is higher than FEM, since the construction of the RK basis functions requires solving reproducing equations at each integration point.

The Radial Basis function (RBF) has been introduced as the bases for approximation and exhibit exponential convergence rate [31]. Taking derivatives of RBFs for PDEs requires relatively smaller effort compared to other approximation functions. Kansa [32-33] first applied RBFs to solve PDEs. Franke and Schaback [34] and Wendland [35] gave the theoretical foundation of RBFs for solving PDEs. Hu et al. [36-37] introduced RBFs with collocation methods to solve elliptic boundary value problems. Although the RBF approximation shows excellent performance with respect to accuracy, it yields a full matrix and exhibits ill-conditioning as the model is refined. To avoid the issues encountered in the RBF approximation, Chen et al. [38] introduced the RK approximation as the localization function of the RBF under partition of unity framework to enhance the stability of BRF. This work combined the advantages of the RBF and RK functions to yield a local approximation that is better conditioned than that of the RBF approximation, while offering a higher rate of
convergence than that of the RK functions.

In this work, we introduce the RK and RBF approximations to the discretization of random spaces. By taking advantages of the polynomial reproducibility and local approximation in the RK approximation, better accuracy and stability in the approximation of random variables are achieved. The exponential convergence property of RBFs also makes it an excellent candidate for approximation of random variables. However, for multi-dimensional problems, the computational cost grows dramatically as the dimensionality increases. The Smolyak algorithm [39] is used to make the optimal choices of the sets of collocation points. Furthermore, by discretizing the random space with uniform point distributions, the RK approximation in one-dimension only need to be formed at minimal points, and the multi-dimensional RK approximation can be constructed by the tensor product of the one-dimensional RK functions. We utilize this tensor product formulation and propose the algorithms for the linear system to be decomposed and solved in each dimension. These accelerated algorithms will be applied to solutions of stochastic PDEs by using the RK and RBF approximations.

### 2.3 Overview for the Modeling of Crack Propagation

In the literature, the extended finite element method (X-FEM) has been popularly selected in fracture mechanics to model crack propagation [40-44]. The displacement field near the crack surface is represented by extrinsically enriching the original nodal shape functions, which exploits the partition of unity (POU) property of finite elements [45]. Mesh-free methods [46-53] are also developed for modeling fracture and crack growth. Krysl and Belytschko [51] proposed a so-called "visibility" criterion to account for the discontinuity near the crack tip, in which the nodal domain of influence is simply truncated based on the alignment of crack
tip and node. Another near-tip enrichment with so-called "diffraction" criterion was proposed to avoid the discontinuities stemming from the visibility criterion [48-49]. The smoothed shape functions are constructed such that their influence bends around the tip of a crack similar to the way light diffracts around a sharp corner. Fleming et al. [50] proposed intrinsic enrichment schemes to represent the discontinuity and singularity of the near-tip field by embedding the analytical asymptotic solutions of the crack tip field to the basis of the Moving Least Squares approximation.

The modeling of the dynamic crack propagation has been discussed under the framework of X-FEM [54-58]. Réthoré et al. [54] proposed an enrichment strategy which satisfies the stability conditions and also ensures energy conservation with implicit time integration scheme. In this paper, a technique is proposed based on Lagrangian conservation for the estimation of dynamic stress intensity factors for arbitrary 2D cracks. Menouillard et al. [55] proposed a time-dependent near-tip enrichment method to improve the accuracy of the dynamic stress intensity factors. Belytschko et al. [56] developed a method using the loss of hyperbolicity as a criterion for dynamic crack propagation. To enable both the crack speed and crack direction to be determined for a given material model the criterion of loss of hyperbolicity is tracked by a hyperbolicity indicator. For explicit time integration, mass lumping strategies were proposed by Menouillard et al. [57-58] for modeling dynamic crack propagation. The stability analyses were also conducted based on explicit integration schemes and their proposed mass lumping strategies. For classical theories on dynamic fracture mechanics, one can find more details in the literature [59-62].

In this dissertation, the extrinsically enriched RK shape functions are introduced to model the crack propagation [63]. The off-tip field is represented by enriching the RK shape
functions with Heaviside functions and the near-tip field is modeled by utilizing the visibility criterion [48-49] while preserving the POU property for the enriched RK approximation function. Since the POU property is preserved, the mass remains conservative while other generalized enrichment schemes result in inconsistent nodal masses (the enriched nodes may have different units from non-enriched nodes and the mass of the discretized system changes when the crack propagates). When the crack propagates, new bases for the approximation fields will be introduced. The coefficients of the new bases can be determined by imposing the conservation laws of linear momentum and kinetic energy on the enriched nodes without solving the equations of motion. Consequently, the computational complexity can be reduced. The proposed methods will be verified by two benchmark problems for dynamic linear elastic fracture mechanics.

More details of classical theories of linear elastic fracture mechanics (LEFM) can be found in the literature. Irwin [64] derived the asymptotic displacement and stress fields near the crack tip based on the compatibility and equilibrium conditions in linear elasticity. Rice [65] proposed a path independent contour integral, named the $J$-integral, as the criterion of crack propagation. The $J$-integral was then proven to be equal to the fracture energy release rate under the framework of linear elastic fracture mechanics. Attigui and Petit [66] proposed a method to separate the mixed intensity factors by introducing kinematically admissible auxiliary displacement fields to the $J$-integral, as a mix-mode fracture is involved in the concerned fracture problems. In general, LEFM is only applicable when the size of the fracture process zone (FPZ) at the crack tip is small compared to the size of the crack and the size of the specimen [67]. Due to the limitation of LEFM, the cohesive zone model was proposed by Dugdale [68] and Barenblatt [69] for brittle materials. Numerically, the cohesive zone model can also be regarded as a means to regularize the singularity of the near-tip stress
field in LEFM, since in the real material there should no singular stress at the crack tip.

### 2.4 Overview of Multi-scale Methods

Multi-scale modeling has been widely used in many fields, such as mechanics, physics, chemical science, meteorology, computer science, etc. In mechanics, the multi-scale modeling has been applied to homogenization of microstructures such as composite materials [70-71], porous media [72-73], and crystallites [74-76]. The multi-scale methods seek to provide a framework for bridging the physics at different length scales, and offer a new insight into complex phenomena that otherwise cannot be described by the single scale fundamental physics. In the field of multi-scale mechanics of materials, efforts have been made, through the observation of the microstructure behaviors, to relate the mechanics at microscopic level to the mechanics of macroscopic continua. In the multi-scale modeling, asymptotic expansion method [77-78] has been introduced to relate physical variables defined at different scales. The method yields a mathematical framework to obtain the homogenized material properties by solving characteristic functions on a representative cell. Upon obtaining the characteristic functions that couple the coarse scale variables to fine scale variables, the homogenized microstructure properties are mathematically derived and applied to macrostructure systems.

In continuum mechanics, the mathematical description of material inelastic behavior such as plasticity and damage models are phenomenological. However, this continuum description of material laws lacks a connection to the underlined physics at smaller length scale. In recent years, multi-scale modeling has been introduced into the mechanics of inelasticity, for example, the damage mechanics. Lee et al. [79] proposed a hierarchical
multi-scale model to relate the evolution of damages at the macro and micro scales. Fish et al. [80] developed a non-local theory for describing damage phenomena based on two-scale asymptotic expansion. Due to the high computational cost in solving the characteristic functions in the asymptotic expansion type approach, Dascalu et al. [81] constructed damage laws based on micro-mechanical energy balance on representative elementary volume with evolving micro-cracks. Ren and Chen et al. [82] constructed micro-cracks informed damage models based on a energy bridging method, in which damage evolution is treated as a consequence of micro-crack propagation. Fish and Yuan [83] proposed a multi-scale enrichment scheme based on partition of unity (MEPU). In their research, the coarse scale approximation is extrinsically enriched by the fine-scale solutions by utilizing the partition of unity property of the finite element approximation.

Due to the randomness of microstructures, the above mentioned multi-scale modeling requires further extension with consideration of uncertainties. The early work in the stochastic micro-mechanical modeling is the parallel element model [84-86]. This model was proposed to describe the progressive damage evolution of a brittle rod subjected to uniaxial loading. Xu [87] employed polynomial chaos expansions combined with stochastic Galerkin and stochastic collocation methods to formulate the multi-scale methods. Ganapathysubramanian and Zabaras [88] developed a stochastic variational multi-scale formulation to incorporate uncertainties with multi-scale features for modeling flow through random heterogeneous porous media.

A more general framework called stochastic representative volume element (SRVE) methods were proposed for considering the heterogeneity of the microstructures, which are, in fact, prevalent in real materials. The methods under this category aim to provide the foundations from the standpoint of statistical physics directly to the level of the representative
volume element (RVE). Hill [89] defined the concept of RVE as a microscopic cell contains a
very large (mathematically infinite) set of micro-scale elements (e.g. grains) and possesses
statistical homogeneity and ergodic properties. Hazanov [90] discussed the role of Hill's
principle and its applications in modern micromechanics of industrial composite materials.
The Hill condition was generalized for arbitrary materials, in particular for nonlinear inelastic
composites with imperfect interfaces. Huget [91-92] derived the upper and lower bounds of
the effective modulus and compliance tensors by partitioning the domain of microstructure,
which is named partition theorem by Huget. As the concerned domain is smaller than the size
of RVE, the maximum error of the approximated effective modulus can be estimated. With a
similar approach to the partition theorem proposed by Huget, Ostoja-Starzewski [93]
proposed a technique of scale separation to define a RVE. Xu and Graham-Brady [94]
develop a stochastic computational method to evaluate global effective properties and local
probabilistic behavior of random elastic media based on the stochastic decomposition of
random field and the iterative algorithm that takes advantage of fast Fourier transformation.

The objective of the stochastic multi-scale modeling is to obtain the homogenized
macro-scale properties with the consideration of randomness stemmed from the heterogeneity
in the microstructures. This field is still in its infancy and much work needs to be done for
reliable uncertainty quantification of mechanics of materials beyond the deterministic
mathematical models.
Chapter 3

Basic Equations in Stochastic Methods

3.1 Stochastic Boundary Value Problems

Let \((\Omega, \mathcal{F}, P)\) be a complete probability space, in which \(\Omega\) is the event space, \(\mathcal{F} \subset 2^\Omega\) is the \(\sigma\)-algebra of an event, and \(P\) is the probability measure. Consider the bounded domain, \(D \subset \mathbb{R}^d\) with boundary \(\partial D\) and \(\bar{D} = D \cup \partial D\). For a stochastic differential equation, find the stochastic function \(u \equiv u(\theta, x)\): \(\Omega \times \bar{D} \rightarrow \mathbb{R}\), such that for \(P\) almost everywhere in \(\Omega\), the following equation holds:

\[
\Lambda u(\theta, x) = f(\theta, x), \quad x \in D
\]

with the following boundary conditions:

\[
\Gamma u(\theta, x) = g(\theta, x), \quad x \in \partial D
\]

where \(x\) is the vector of coordinates in \(\mathbb{R}^d\), \(\theta\) is the argument in probability space, \(\Lambda\) is a linear differential operator and \(\Gamma\) is the boundary operator. In general, the operators \(\Lambda\) and \(\Gamma\) as well as the driving terms \(f\) and \(g\), are all assumed to involve random variables.

3.2 The Karhunen-Loève Expansion

In numerical analyses, incorporating stochastic process is an important task when uncertainty becomes critical to physical problems. For a random variable \(\alpha\) in terms of the spatial
coordinates, it can be considered as an infinite linear combination of orthogonal functions:

\[ \alpha(x, \theta) = \sum_{n=0}^{\infty} \sqrt{\lambda_n} \xi_n(\theta) f_n(x) \quad (3.3) \]

where \( \alpha \) is a random variable with zero mean, \( \theta \) is the argument in probability space, \( \xi_n(\theta) \) are assumed to be independent random variables, \( \lambda_n \) and \( f_n(x) \) are eigenvalues and eigenfunctions, respectively, to be determined. Since \( \alpha \) is zero mean, \( \xi_n(\theta) \) are also defined with zero mean.

The covariance function of \( \alpha \) is defined as:

\[ C_{\alpha\alpha}(x_1, x_2) = \langle \alpha(x_1, \theta) \alpha(x_2, \theta) \rangle \]
\[ = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \langle \xi_m(\theta) \xi_n(\theta) \rangle \sqrt{\lambda_m \lambda_n} f_m(x_1) f_n(x_2) \quad (3.4) \]

where \( \langle \bullet \rangle \) is the average operator with respect to the probability domain,

\[ \langle \xi_m(\theta) \xi_n(\theta) \rangle = \int_{-\infty}^{\infty} \xi_m(\theta) \xi_n(\theta) P(\xi_m, \xi_n) d\xi_m d\xi_n \quad (3.5) \]

in which \( P(\xi_m, \xi_n) \) is probability density function for the coincidence of \( \xi_m \) and \( \xi_n \).

Assume \( \alpha \) consists of infinite independent events and each event has zero mean, i.e.,

\[ \langle \xi_m(\theta) \xi_n(\theta) \rangle = \delta_{mn} \quad (3.6) \]

Then (3.4) can be rewritten as:

\[ C_{\alpha\alpha}(x_1, x_2) = \sum_{n=0}^{\infty} \lambda_n f_n(x_1) f_n(x_2) \quad (3.7) \]

where \( \{ f_n(x) \} \) is a set of orthogonal functions that are normalized as:

\[ \int_{\Omega} f_m(x) f_n(x) d\Omega = \delta_{mn} \quad (3.8) \]

\( \lambda_n \) and \( f_n(x) \) can be determined by calculating the following integrand:

\[ \int_{\Omega} C_{\alpha\alpha}(x_1, x_2) f_n(x_1) d\Omega_1 = \int_{\Omega} \sum_{m=0}^{\infty} \lambda_m f_m(x_1) f_n(x_2) f_m(x_1) d\Omega_1 = \lambda_n f_n(x_2) \quad (3.9) \]
Given the covariance function \( C_{\alpha\alpha} \), \( \lambda_n \) and \( f_n(x) \) can be obtained with the above technique.

For example, consider a 1-D problem where the covariance function is an exponential function at any two points \( x_1 \) and \( x_2 \):

\[
C_{\alpha\alpha}(x_1, x_2) = \sigma^2 e^{-|x_1-x_2|/b} \tag{3.10}
\]

where \( \sigma \) is a constant and \( b \) is the correlation length defining the relationship of \( \alpha \) between any two points \( x_1 \) and \( x_2 \) within the domain \([-a, a]\). Substituting (3.10) into (3.9), we have

\[
\int_{-a}^{a} C_{\alpha\alpha}(x_1, x_2) f_n(x_1) \, dx_1 = \int_{-a}^{a} \sigma^2 e^{-|x_1-x_2|/b} f_n(x_1) \, dx_1 = \lambda_n f_n(x_2) \tag{3.11}
\]

Differentiating both sides of (3.11) twice with respect to \( x_2 \), the following eigen-equation can be derived:

\[
\lambda_n f_n^{\prime\prime}(x_2) + \left[ (2\sigma^2 + \lambda_n)/b \right] f_n(x_2) = 0 \tag{3.12}
\]

and denoting \( \omega_n^2 = (2\sigma^2 + \lambda_n)/b \), (3.12) can be expressed as:

\[
\lambda_n f_n^{\prime\prime}(x) + \omega_n^2 f_n(x) = 0 \tag{3.13}
\]

Solving (3.13), the following equations can be derived:

\[
\frac{1}{b} - \omega_n \tan(\omega_n a) = 0 \tag{3.14}
\]

\[
\omega_n + \frac{1}{b} \tan(\omega_n a) = 0 \tag{3.15}
\]

Denoting the solutions of (3.14) and (3.15) as \( \omega_n \) and \( \omega_n^* \), respectively, the eigen-functions are:

\[
f_n(x) = \frac{\cos(\omega_n x)}{\sqrt{a + \frac{\sin(2\omega_n a)}{2\omega_n}}} \tag{3.16}
\]
As $a=0.5$ and $b=1.0$:

\[ f_n^*(x) = \frac{\sin(\omega_n^* x)}{\sqrt{a - \sin(2\omega_n^* a)/2\omega_n^*}} \quad (3.17) \]

\[ \alpha(x, \theta) = \sum_{n=0}^{\infty} \sigma \sqrt{\mu_n^* \xi_n(\theta)} f_n^*(x) \quad (3.18) \]

\[ \begin{align*}
\omega_1 & = 1.306542374 \\
\omega_2 & = 6.584620043 \\
\omega_3 & = 12.72324078 \\
\omega_4 & = 18.95497141 \\
\omega_5 & = 3.673194406 \\
\omega_6 & = 9.631684636 \\
\omega_7 & = 15.83410537 \\
\omega_8 & = 22.08165964 \\
\end{align*} \]

\[ \mu_n = \frac{2}{\omega_n^*} + 1 \quad \mu_n^* = \frac{2}{\omega_n^{*2}} + 1 \quad (3.19) \]

The comparison between the exact covariance function and the approximation with 4-term (\( \omega_1^*, \omega_2^* \) and \( \omega_3^*, \omega_4^* \)) Karhunen-Loève expansion is shown in Figure 3.1.

**Figure 3.1 The plots of exponential covariance function**
3.3 The Monte Carlo Simulation

The procedure of the Monte Carlo simulation for the stochastic analysis is as follows:

a. Sampling through a large number of possible values of the input random parameters.

b. Substituting the possible values of the input parameters into the deterministic system to determine their respective output data:

c. Processing all the output data to obtain the statistical properties.

The Monte Carlo method is the most popular approach to solve a stochastic problem because of its simplicity. Such approach is simple but time consuming, since sufficient simulations are required for obtaining reliable information of the stochastic analysis. The convergence of the Monte Carlo method has been proved to be in the order of $1/\sqrt{N}$ for the mean value by using the Central Limit Theorem [97]:

$$e = \left| \bar{D}_{MC} - \bar{D} \right| \approx \sigma_o \frac{1}{\sqrt{N}}$$ \hspace{1cm} (3.21)

where $\bar{D}$ is the exact mean of the random function $D$ and $\bar{D}_{MC}$ is the numerical mean value obtained by using Monte Carlo methods, $\sigma_o$ is the standard deviation of $D$ and $N$ is the number of samples. The proof is shown as follows:

The error of mean by using MC methods can be defined as

$$e = \left| \bar{D}_{MC} - \bar{D} \right| = \sqrt{\left( \bar{D}_{MC} - \bar{D} \right)^2} = \sqrt{\left( \frac{1}{N} \sum_{k=1}^{N} D(\xi_k) - \bar{D} \right)^2}$$ \hspace{1cm} (3.22)

Further expanding the above equation, we have

$$e = \frac{1}{N^2} \left( \sum_{k=1}^{N} (D(\xi_k) - \bar{D}) \sum_{l=1}^{N} (D(\xi_l) - \bar{D}) \right)$$ \hspace{1cm} (3.23)

Since $\xi_k$ and $\xi_l$ are independent events, if $k \neq l$,
Using (3.24), (3.23) can be re-arranged as

$$e = \sqrt{\frac{1}{N^2} \left( \sum_{k=1}^{N} (D(\xi_k) - \bar{D})(D(\xi_i) - \bar{D}) \right)}$$

$$\approx \sigma_D \frac{1}{\sqrt{N}}$$

(3. 25)

Although the convergence of Monte Carlo methods is slow, Monte Carlo methods are still good approaches as the concerned stochastic problems are highly dimensional. Note that the convergence of Monte Carlo methods is independent of the dimensionality of the random variables, while for some other methods requiring cubature rules the dimensionality will exponentially increase the computational cost that will be discussed later. To reduce the computational cost, some techniques were introduced to accelerate Monte Carlo methods, such as the variance reduction methods [98], transformation methods [99], acceptance-rejection method [100], reweighting approach [101], and importance sampling [102]. In this dissertation we use the Monte Carlo simulation to generate a reference solution for comparison with other stochastic methods.

### 3.4 The Neumann Expansion

In general, stochastic systems involving a linear differential equation can be expressed as:

$$\Lambda u = f$$

(3. 26)

where $\Lambda$ is a linear stochastic differential operator, $u$ is the random response, and $f$ can be considered as a random excitation. The stochastic differential operator can be further decomposed into two parts:

$$\Lambda = L + \Pi$$

(3. 27)

where $L$ is the deterministic operator and $\Pi$ is the random operator:
(L + \Pi) \ u = f \quad (3.28)

By calculating the inverse of the operator L, the stochastic system can be solved. Assuming the inverse of the operator L exists, (3.28) can be expressed as:

\[ u = L^i f - L^i \Pi u \quad (3.29) \]

Substituting (3.29) into the right-hand side of the equation:

\[ u = L^i f - L^i \Pi L^i f + L^i \Pi L^i \Pi u \quad (3.30) \]

Through substituting (3.29) into the above expansion recursively, the random response \( u \) can be expressed as an infinite series in terms of the differential operators and the excitation:

\[ u = \sum_{i=0}^{\infty} \frac{(-1)^i}{i!} \left( L^i \Pi \right) \left( L^i f \right) \quad (3.31) \]

Note that (3.31) is valid only if the following condition is satisfied:

\[ \| L^i \Pi \| < 1 \quad (3.32) \]

We will discuss the connection between the Neumann expansion and the Taylor series expansion. Consider a first order differential equation:

\[ \frac{dy(x)}{dx} = -ky(x), \quad y(0) = 1, \quad x \in [0,1] \quad (3.33) \]

where the coefficient \( k \) is considered to be a random variable \( k(\theta) \) with Gaussian distribution and its mean is 0 and variance is 1. The solution of (3.33) is

\[ y(k, x) = \exp(-kx) \quad (3.34) \]

The following derivation shows the process to solve (3.34) with the Neumann expansion:

Firstly, decompose the function \( y(x) \) into two parts:

\[ y(x) = \overline{y}(x) + y(0), \quad \overline{y}(0) = 0 \quad (3.35) \]

Substitute (3.35) into (3.33) to yield

\[ \frac{d\overline{y}(x)}{dx} + k\overline{y}(x) = -ky(0) \quad (3.36) \]

Applying the Neumann expansion, we have
Then the solution of (3.33) can be expressed as

\[ y(x) = y(0) \left\{ -k (x + C_1) + k^2 \left( \frac{x^2 + C_1 x + C_2}{2} \right) - k^3 \left( \frac{x^3}{6} + C_1 \frac{x^2}{2} + C_2 x + C_3 \right) + ... \right\} \]  (3.38)

Since \( k \) is arbitrary and \( \bar{y}(0) = 0 \), all the constants \( C_i \) should be 0. Hence

\[ \bar{y}(x) = y(0) \left\{ -kx + \frac{(kx)^2}{2} - \frac{(kx)^3}{6} + \frac{(kx)^4}{24} - ... \right\} \]  (3.39)

The solution of (3.33) by employing the Neumann expansion is

\[ y(x) = \bar{y}(x) + y(0) \]

\[ = \bar{y}(x) = y(0) \left\{ 1 - kx + \frac{(kx)^2}{2} - \frac{(kx)^3}{6} + \frac{(kx)^4}{24} - ... \right\} \]  (3.40)

Comparing (3.40) to (3.34), the Neumann expansion and the Taylor series expansion generate identical solutions as demonstrated below:

\[ y(0) \exp(-kx) = y(0) \left\{ 1 - kx + \frac{(kx)^2}{2} - \frac{(kx)^3}{6} + \frac{(kx)^4}{24} - ... \right\} \]  (3.41)

### 3.5 Stochastic Galerkin and Collocation Methods

By taking the Galerkin approximation in \( D \) for (3.1), the solution is projected to the space spanned by a test function \( v(x) \):

\[ \langle v(x), Lu(\theta,x) \rangle_D = \langle v(x), f(\theta,x) \rangle_D \]  (3.42)

where \( \langle \cdot, \cdot \rangle_D \) is the integration operator over the domain \( D \). Using the weak formulation, the equation can be transformed to a discrete form:

\[ K(\theta)U(\theta) = F(\theta) \]  (3.43)
where $K$, $U$ and $F$ contain the random variable, $\theta$.

$$
K(\theta) = \begin{bmatrix}
K_{11}(\theta) & K_{12}(\theta) & \cdots & K_{1N}(\theta) \\
K_{21}(\theta) & K_{22}(\theta) & \cdots & K_{2N}(\theta) \\
\vdots & \vdots & \ddots & \vdots \\
K_{N1}(\theta) & K_{N2}(\theta) & \cdots & K_{NN}(\theta)
\end{bmatrix}
$$

(3.44)

$$
U(\theta) = \langle U^1(\theta) \ U^2(\theta) \ \cdots \ U^N(\theta) \rangle \\
F(\theta) = \langle F^1(\theta) \ F^2(\theta) \ \cdots \ F^N(\theta) \rangle
$$

and

$$
u(\theta, x) = \sum_{i=1}^{N} N^i(x) \ U^i(\theta) \quad (3.45)$$

In the discrete equations, each component in the vector $U$ involves randomness to be computed. If the probability space can be further characterized by a finite number of random variables $\xi$, (3.43) can be rewritten in the following form:

$$
K(\xi(\theta)) U(\xi(\theta)) = F(\xi(\theta)) \quad (3.46)
$$

where $\xi(\theta) = (\xi_1(\theta), \xi_2(\theta), \ldots, \xi_M(\theta))$ are assumed to be independent events, each is equipped with probability density functions $\rho_i(\xi_i(\theta))$. Note that the random variables $\xi$ are required to be independent.

By solving (3.46), the mean and covariance matrix of $U$ can be determined by taking expectation of the solution vector $U$:

$$
U = \hat{E}(U) = \int_{\Omega} U(\xi) \ \rho_1(\xi_1) \ \rho_2(\xi_2) \ \cdots \ \rho_M(\xi_M) \ d\xi_1 \ d\xi_2 \ \cdots \ d\xi_M \\
R_{UU} = \hat{E}(U, U) = \int_{\Omega} U(\xi) U^T(\xi) \ \rho_1(\xi_1) \ \rho_2(\xi_2) \ \cdots \ \rho_M(\xi_M) \ d\xi_1 \ d\xi_2 \ \cdots \ d\xi_M \quad (3.47)
$$

As shown in (3.46), the linear system is stochastic, and the solution cannot be directly obtained. The generalized polynomial chaos (gPC) was considered to approximate the stochastic solution [21-23]:

$$
U^i(\xi) = \sum_{n=0}^{N} \Psi_n(\xi) a^i_n \quad (3.49)
$$
where \( U^I(\xi) \) is the solution of the \( I \)-th component in \( U(\xi) \), \( \Psi_n(\xi) \) is the \( n \)-th order polynomial function of \( \xi \), \( a^I_n \) are the generalized coefficients of component \( I \) to be determined, and \( N \) is the highest order of the polynomial basis functions. The 0-th order basis function is given as

\[
\Psi_0(\xi) = 1 
\]

The basis functions of gPC are constructed to be orthogonal with respect to the probability density function \( \rho(\xi) \) in the random space:

\[
E(\Psi_k(\xi)\Psi_L(\xi)) = \int_{\Omega} \rho(\xi)\Psi_k(\xi)\Psi_L(\xi)d\xi = \begin{cases} 0, & K \neq L \\ c_k \neq 0, & K = L \end{cases} \quad (3.51)
\]

With a set of orthogonal basis functions, the coefficients in the stochastic approximation of (3.49) is obtained from the Galerkin weak form of (3.51), and then the mean and variance of the solution can be easily determined:

\[
\text{mean} = E\left(U^I(\xi)\right) = a_0 \\
\text{variance} = E\left(\left(U^I(\xi)\right)^2\right) = \sum_{n=0}^{N} c_n a_n^2 \quad (3.52)
\]

The stochastic linear system in (3.46) can also be solved by collocation method [103], where the solution at a collocation point \( \xi^k = (\xi^k_1, \xi^k_2, \ldots, \xi^k_M) \) is obtained by

\[
U(\xi^k) = K^{-1}(\xi^k)F(\xi^k) \quad (3.53)
\]

Upon obtaining the solution of (3.46) at collocation points, we have the following relation:

\[
U^I(\xi) = \sum_{n=1}^{N_I} \Psi_n(\xi) a^I_n \quad (3.54)
\]

Consequently, we have the following linear equation for solving the coefficients of approximation:
where $N_c$ is the number of the collocation points. If $N_c > N_s$, (3.55) becomes an overdetermined system, which can be solved by using the least-squares method. Define a least-squares functional of the residual, $\mathbf{e} = \mathbf{B}a' - \mathbf{u}'$ as:

$$\Pi = \frac{1}{2} \| \mathbf{e} \|^2 = \frac{1}{2} \mathbf{e}^T \mathbf{e} = \frac{1}{2}(\mathbf{B}a' - \mathbf{u}')^T(\mathbf{B}a' - \mathbf{u}')$$  \hspace{1cm} (3.56)

Minimizing $\Pi$ requires:

$$\frac{\partial \Pi}{\partial a_i} = \mathbf{B}^T(\mathbf{B}a' - \mathbf{u}') = 0$$  \hspace{1cm} (3.57)

or

$$\mathbf{B}^T\mathbf{B}a' = \mathbf{B}^T\mathbf{u}'$$  \hspace{1cm} (3.58)

Note that the stochastic collocation method requires solving the deterministic systems repeatedly, which can be performed in parallel.

Nowadays, the stochastic collocation methods are becoming popular for stochastic analysis because of the ease of implementation. The methods incorporate the benefits of Monte Carlo methods and function approximation schemes. Through sampling a set of referenced points, the solution can be determined by function approximation schemes based on the information at the collocation points. In contrast to the stochastic Galerkin methods, the stochastic collocation methods require solving many smaller deterministic systems rather than solving a large system through expanding the stochastic linear system. The deterministic system can be solved by purely parallel solvers without any extra effort on communication between these solvers. However, for stochastic Galerkin methods, the resulting equations for
the expansion coefficients are coupled, hence the numerical algorithm needs to deal with a larger, coupled system. Using stochastic Galerkin methods will be computationally expensive and require larger memory for storing the expanded matrix. Consequently the stochastic collocation methods show better efficiency than Galerkin methods; the concern now turns to the accuracy of the stochastic collocation methods.

For stochastic Galerkin methods, the coefficients are determined by constructing orthogonal basis functions and projecting the solution to the set of orthogonal functions. Such scheme ensures the residual of the stochastic governing equation orthogonal to the linear space spanned by these basis functions, hence it optimizes the accuracy. In contrast, for stochastic collocation methods, the solution has already inherited errors from the approximation scheme in the spatial domain. As the solution is further approximated in the probability domain, especially for multi-dimensional stochastic problems, the errors become more significant. These errors are classified as aliasing errors. Consequently, the approximation in the special domain for solving the deterministic system in (3.46) requires higher accuracy than the one used in the stochastic Galerkin methods.

### 3.6 The Homogeneous Chaos

The homogeneous chaos expansion employs the Hermite polynomials in terms of Gaussian random variables [17]. According to Cameron and Martin, the Fourier-Hermite series converge to any L₂ functional in the L₂ sense. This means the homogeneous chaos expansion converges to any processes with finite second-order moments. Since the bases of the homogeneous chaos are orthogonal with respect to the Gaussian distribution, the theory is under the category of the generalized polynomial chaos (gPC). A random variable \( \mu(\theta) \) can be expressed as a polynomial series of independent events:
\[ \mu(\theta) = a_0 \Gamma_0 + \sum_{\xi=1}^{\infty} a_\xi \Gamma_1 \left( \xi_{\xi}(\theta) \right) + \sum_{\xi=1}^{\infty} \sum_{\xi=1}^{\xi} a_{\xi\xi} \Gamma_2 \left( \xi_{\xi}(\theta), \xi_{\xi}(\theta) \right) + \ldots \] (3.59)

In (3.59), \( \Gamma_0, \Gamma_1, \Gamma_2, \Gamma_3 \ldots \) are defined as independent events constructed by the bases of the Gaussian random variables \( \xi_n(\theta) \):

\[ \langle \Gamma_i, \Gamma_j \rangle = 0, \quad \text{if} \quad i \neq j \]
\[ \neq 0, \quad \text{if} \quad i = j \] (3.60)

and

\[ \langle \Gamma_i \rangle = 0, \quad \text{if} \quad i \neq 0 \] (3.61)

To satisfy the conditions of (3.60) and (3.61), the general expression of the polynomials is given by:

\[ \Gamma_n(\xi_1, \ldots, \xi_n) = e^{\frac{1}{2} \xi_1^2} \frac{\partial^n}{\partial \xi_1^n} - e^{\frac{1}{2} \xi_1^2} \] (3.62)

According to Favard’s theorem [104], all the orthogonal polynomials on the real line satisfy a three-term recurrence relation. Consider a sequence of polynomials \( \{ P_n(x) \} \) in which \( n \) denotes the order of the polynomial, the following equation is used to impose the orthogonal conditions,

\[ P_n(x) = (x - c_n) P_{n-1}(x) - \lambda_n P_{n-2}(x) \] (3.63)

where \( c_n \) and \( \lambda_n \) are constants which need to be determined. To satisfy the orthogonal conditions, we need

\[ \langle P_n(x) P_{n-1}(x) \rangle = 0 = \langle (x - c_n) P_{n-1}(x) P_{n-1}(x) \rangle - \langle \lambda_n P_{n-2}(x) P_{n-1}(x) \rangle \]

\[ = \langle (x - c_n) P_{n-1}(x) P_{n-1}(x) \rangle \] (3.64)

\[ \langle P_n(x) P_{n-2}(x) \rangle = 0 = \langle (x - c_n) P_{n-1}(x) P_{n-2}(x) \rangle - \langle \lambda_n P_{n-2}(x) P_{n-2}(x) \rangle \]

\[ = \langle x P_{n-1}(x) P_{n-2}(x) \rangle - \langle \lambda_n P_{n-2}(x) P_{n-2}(x) \rangle \] (3.65)

Then, the coefficients \( c_n \) and \( \lambda_n \) are

28
For $j$-th order component of \( \{ P_n(x) \} \), where $j < n-2$

\[
\langle P_n(x) P_j(x) \rangle = 0 = \langle (x - c_j) P_{n-1}(x) P_j(x) \rangle - \langle \lambda_n P_{n-2}(x) P_j(x) \rangle = \langle (x - c_j + c_j - c_n) P_{n-1}(x) P_j(x) \rangle \tag{3.68}
\]

Substitute the recursive condition of (3.63) into (3.68) to yield

\[
\langle P_n(x) P_j(x) \rangle = \langle (P_{j+1}(x) + \lambda_j P_{j-1}(x)) (c_j - c_n) P_{n-1}(x) \rangle = (c_j - c_n) \langle P_{j+1}(x) P_{n-1}(x) \rangle + \lambda_j (c_j - c_n) \langle P_{j-1}(x) P_{n-1}(x) \rangle = 0 \tag{3.69}
\]

Hence, if \( \{ P_n(x) \} \) satisfies the recursive relation with $n$ starting from 0-th order, the sequence of polynomials satisfies the orthogonal conditions of (3.60).

Table 3.1 and Table 3.2 list the orthogonal polynomials with Gaussian probability distribution for one and two dimensional cases. They can be derived directly from (3.62).

**Table 3.1: One dimensional polynomial chaos**

<table>
<thead>
<tr>
<th>term $j$</th>
<th>Order $i$</th>
<th>$\Gamma_j = \hat{\Gamma}_j$</th>
<th>$\langle \Gamma_j ^2 \rangle$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>$\xi_i$</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>$\xi_i^2 - 1$</td>
<td>2</td>
</tr>
<tr>
<td>3</td>
<td>3</td>
<td>$\xi_i^3 - 3\xi_i^2$</td>
<td>6</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>$\xi_i^4 - 6\xi_i^3 + 3$</td>
<td>24</td>
</tr>
</tbody>
</table>
### Table 3.2(a): Two dimensional polynomial chaos

<table>
<thead>
<tr>
<th>Term $j$</th>
<th>Order $i$</th>
<th>$\Gamma_i (= \hat{\Gamma}_j)$</th>
<th>$\langle \Gamma_i^2 \rangle$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>$\xi_1$</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>$\xi_2$</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>$\xi_1^2 - 1$</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>2</td>
<td>$\xi_1 \xi_2$</td>
<td>1</td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>$\xi_2^2 - 1$</td>
<td>2</td>
</tr>
<tr>
<td>6</td>
<td>3</td>
<td>$\xi_1^3 - 3 \xi_2^2$</td>
<td>6</td>
</tr>
</tbody>
</table>

### Table 3.2(b): Two dimensional polynomial chaos (continued)

<table>
<thead>
<tr>
<th>Term $j$</th>
<th>Order $i$</th>
<th>$\Gamma_i (= \hat{\Gamma}_j)$</th>
<th>$\langle \Gamma_i^2 \rangle$</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>3</td>
<td>$\xi_1^3 \xi_2 - \xi_2^3$</td>
<td>2</td>
</tr>
<tr>
<td>8</td>
<td>3</td>
<td>$\xi_1 \xi_2^2 - \xi_2^3$</td>
<td>2</td>
</tr>
<tr>
<td>9</td>
<td>3</td>
<td>$\xi_2^3 - 3 \xi_2^3$</td>
<td>6</td>
</tr>
<tr>
<td>10</td>
<td>4</td>
<td>$\xi_1^4 - 6 \xi_2^3 + 3$</td>
<td>24</td>
</tr>
<tr>
<td>11</td>
<td>4</td>
<td>$\xi_1^3 \xi_2 - 3 \xi_1 \xi_2^2$</td>
<td>6</td>
</tr>
<tr>
<td>12</td>
<td>4</td>
<td>$\xi_1^2 \xi_2^2 - \xi_1^2 - \xi_2^2 + 1$</td>
<td>4</td>
</tr>
<tr>
<td>13</td>
<td>4</td>
<td>$\xi_1^3 \xi_2^3 - 3 \xi_1^2 \xi_2^3$</td>
<td>6</td>
</tr>
<tr>
<td>14</td>
<td>4</td>
<td>$\xi_2^4 - 6 \xi_2^3 + 3$</td>
<td>24</td>
</tr>
</tbody>
</table>

### 3.7 Selection of Collocation Points by using the Smolyak Algorithm

Employing collocation methods to solve the stochastic differential equations necessitates
optimal selection of collocation points. For multi-variate functions, the computational complexity increases exponentially with respect to the dimensionality. In the Smolyak algorithm [39], the approximation of a multi-variate function is formulated by optimizing the combination of one-dimensional approximations.

Assume that a multi-dimensional function $f$ can be expressed as a tensor product of one-dimensional functions:

$$
 f(x_1, x_2, ..., x_d) \approx f_1(x_1)f_2(x_2)....f_d(x_d) \\
 = f_1(x_1) \otimes f_2(x_2) \otimes .... \otimes f_d(x_d) \\
 \equiv \otimes_{k=1}^{d} f_k(x_k)
$$

(3.70)

where $\otimes$ is the tensor product operator and $d$ is the dimensionality of $f$.

To approximate $f$, some approximation scheme is employed as

$$
 f^a = S_d(f) 
$$

(3.71)

where $f^a$ is the approximation function of $f$ and $S_d$ is a continuous linear operator.

The linear operator $S_d$ projects $f$ from a real Banach space of functions $f$ (denoted as $F_d$) to a real Hilbert space of functions (denoted as $G_d$):

$$
 S_d : F_d \to G_d
$$

(3.72)

Assume $S_d$, $F_d$ and $G_d$ can also be separated as a tensor product of one-dimensional linear operators and functions:

$$
 S_d = S_1 \otimes S_1 \otimes .... \otimes S_1 = \otimes_{k=1}^{d} S_1
$$

(3.73)

$$
 F_d = F_1 \otimes F_1 \otimes .... \otimes F_1 = \otimes_{k=1}^{d} F_1
$$

(3.74)

$$
 G_d = G_1 \otimes G_1 \otimes .... \otimes G_1 = \otimes_{k=1}^{d} G_1
$$

(3.75)

Then, (3.71) can be expressed as
The approximation algorithms (operators) $U_i$ with $i \geq 1$ is used to approximate the problem \{F_1, G_1, S_1\} for $d=1$, such that

$$\|S_i - U_i\| \to 0 \quad \text{as} \quad i \to \infty$$

(3.77)

where $i$ denotes the level of the approximation scheme so that with the same approximation scheme, the discretization is refined as $i$ increases. Here $\| \cdot \|$ is an operator norm defined as follows:

$$\|A\| = \sup_{f \neq 0} \frac{\|Af\|}{\|f\|_{\infty}}$$

(3.78)

The difference operator $\Delta_i$ of the approximation in one dimension between two subsequent levels $U_i$ and $U_{i-1}$ is defined as:

$$\Delta_i = U_i - U_{i-1}, \quad \Delta_0 = U_0 = 0$$

(3.79)

where the left superscript $i$ denotes the level of the approximation. For convergence, we need:

$$\|\Delta_i\| \to 0 \quad \text{as} \quad i \to \infty$$

(3.80)

The error bound of $\Delta_i$ can be assumed to be

$$\|\Delta_i\| \leq ED^i$$

(3.81)

where $E$ is a finite positive real number, $D$ is a positive real number which is less than 1.

Consider a multi-dimensional approximation formulated by an $N$-th level one-dimensional approximation, (3.76) can then be expressed as:

$$f^a = \bigotimes_{k=1}^{d} S_i(f_k) \approx \bigotimes_{k=1}^{d} U_N(f_k)$$

(3.82)
The one-dimensional approximation $U_N$ can be expressed as the summation of $\Delta_i$ from level 1 to $N$:

$$
U_N = U_N - U_{N-1} + U_{N-1} - U_{N-2} + ... + U_1 - U_0 = \Delta_N + \Delta_{N-1} + \Delta_{N-2} + ... + \Delta_1
$$

(3.83)

Substituting (3.83) into (3.82), the approximation can then be expressed in the following form:

$$
f^a = \sum_{d \leq i_1 + i_2 + ... + i_d \leq Nd} \Delta_{i_1}(f_1) \otimes \Delta_{i_2}(f_2) \otimes ... \otimes \Delta_{i_d}(f_d)
$$

(3.84)

where $Nd$ is the highest order of the combinations. The approximation function can be considered as the linear combination of the operators $\Delta_{it}$ with respect to approximation level $k$. The highest order of the scheme is up to $Nd$. Using (3.81), the error bound of each component in the right-hand side of (3.84) is

$$
\left\| \Delta_{i_1} \Delta_{i_2} ... \Delta_{i_d} \right\| \leq E^d D^{i_1 + i_2 + ... + i_d}
$$

(3.85)

According to (3.85), the number of $(i_1 + i_2 + ... + i_d)$ represents the order of the term in the series of (3.84). Higher order terms contribute less to the approximation scheme compared with the lower order ones. The expression of the approximation in (3.84) ranks the terms in the linear combination of the 1-D algorithms, so that for reducing the computational cost, the higher order terms have top priority to be eliminated. If the highest order is only up to $q$ ($d \leq q \leq Nd$), (3.84) can be modified as

$$
f^a = \sum_{d \leq i_1 + i_2 + ... + i_d \leq q} \Delta_{i_1}(f_1) \otimes \Delta_{i_2}(f_2) \otimes ... \otimes \Delta_{i_d}(f_d) = A(q,d)(f)
$$

(3.86)

where $A(q,d)$ is the linear operator of the approximation scheme.

For example, take a 2-D case with a referenced level $N=3$:...
Expanding (3.87), we have

\[ f'' = \sum_{2 \Delta_i + i_2 \leq 6} \Delta_i (f_i) \otimes \Delta_j (f_j) = A(2,6)(f) \] (3.87)

Expanding (3.87), we have

\[
A(2,6) = \sum_{2 \Delta_i + i_2 \leq 6} \Delta_i \otimes \Delta_j,
\]

\[
= \Delta_1 \otimes \Delta_1 + \Delta_1 \otimes \Delta_2 + \Delta_1 \otimes \Delta_3 + \Delta_2 \otimes \Delta_1 + \Delta_2 \otimes \Delta_2 + \Delta_3 \otimes \Delta_1
\]

(3.88)

Neglecting the higher order terms where \((i_1 + i_2) > q=4\), (3.88) becomes

\[
A(2,4) = \Delta_1 \otimes \Delta_1 + \Delta_1 \otimes \Delta_2 + \Delta_2 \otimes \Delta_1
\]

(3.89)

Using the following relationship between \( \Delta_j \) and \( U_i \)

\[
\Delta_j = U_i - U_{i-1}
\] (3.90)

(3.89) can be rearranged as

\[
A(2,4) = U_1 \otimes U_3 + U_2 \otimes U_2 - U_1 \otimes U_2 + U_3 \otimes U_1 - U_2 \otimes U_1
\] (3.91)

For different levels of the approximation scheme, define various discretizations from coarse to fine as the level goes from low to high within the 1-D occupied domain [-1,1] as illustrated in Figure 3.2.

\[ \Theta_1 : \text{Level 1, 2 nodes} \]

\[ \Theta_2 : \text{Level 2, 3 nodes} \]

\[ \Theta_3 : \text{Level 3: 5 nodes} \]

\[ \Theta_i : \text{Sets of nodes of scheme } U_i : \]

**Figure 3.2** Different levels of discretization for 1-D approximation scheme

By combining the 1-D algorithms in (3.86), the two dimensional approximation is illustrated in Figure 3.3.
Solving (3.91), the order of the approximation of function $f$ is 4. The total required nodes are 17 based on the union of the nodal sets:

$$\Theta_d = \bigcup_{3i_1 + i_2 \leq 4} \Theta_i \times \Theta_i$$ (3.92)

while the full set requires 25 nodes as shown in Fig. 3.3.

In general, the approximation with the highest order $q$ can be derived by substituting (3.79) into (3.86) [39]:

$$f^q = \sum_{d \leq i_1 + i_2 + \ldots + i_d \leq q} \Delta_i(f_1) \otimes \Delta_i(f_2) \otimes \ldots \otimes \Delta_i(f_d)$$

$$= \sum_{q - d + 1 \leq |\mathbf{i}| \leq q} (-1)^{|\mathbf{i}|} \binom{d-1}{q-|\mathbf{i}|} \bigotimes_{k=1}^{d} U_{i_k}(f_k)$$

$$\equiv A(q, d)(f)$$ (3.93)

where $|\mathbf{i}| = i_1 + i_2 + \ldots + i_d$, and

$$\binom{d-1}{q-|\mathbf{i}|} \equiv \frac{(d-1)!}{(d-1) - (q - |\mathbf{i}|)!(q - |\mathbf{i}|)!}$$ (3.94)

is the binomial coefficient.

---

**Figure 3.3** The nodal sets for the combination of 1-D approximation schemes with different levels
Figure 3.4 The number of the required nodes for Somlyak algorithm up to order $q$ and the full set as $q=Nd$
Chapter 4

The Generalized Stochastic Chaos (GSC)

The generalized polynomial chaos (gPC) [21] introduces global polynomials for construction of the orthogonal basis functions. However, the accuracy of such an approximation relies on the increase of the order of the basis functions, causing numerical oscillation when dealing with problems of high nonlinearity or discontinuity. The global polynomial based approximation schemes may converge slowly, as the solution is rough. Some alternatives should be considered for the stochastic problems to ensure the convergence for those highly non-linear or discontinuous problems. This phenomenon will be discussed in the numerical examples. Two existing approximation methods are adopted for approximating the solution in the probability space: the reproducing kernel (RK) and the radial basis function (RBF) approximations.

4.1 The Reproducing Kernel (RK) Approximation

One of the popular choices for constructing approximation series is the Reproducing Kernel approximation. In the stochastic analysis, the discrete RK approximation for a function in terms of random variables $\xi$ is expressed as:

$$ u^h (\xi) = \sum_{i=1}^{N_r} \Psi_i (\xi) d_i $$

(4.1)
where \( N_s \) is the number of the source points (or basis functions), \( d_l \) are the generalized coefficients to be determined, and \( \Psi_j(\xi) \) is the approximation function expressed as:

\[
\Psi_j(\xi) = C(\xi; \xi - \xi_j) \Phi_a(\xi - \xi_j) 
\]

(4.2)

where \( \Phi_a(\xi - \xi_j) \) is the kernel function that introduces the locality of the approximation with a compact support measured by ‘\( a \)’ and defines the smoothness of the approximation function, and \( C(\xi; \xi - \xi_j) \) is a correction function expressed as follows:

\[
C(\xi; \xi - \xi_j) = \sum_{p+q=0}^{n} (\xi_1 - \xi_{1j})^p (\xi_2 - \xi_{2j})^q b_{pq}(\xi)
\]

\[
\equiv H^T(\xi - \xi_j) b(\xi) 
\]

(4.3)

where \( n \) refers to the order of completeness in this approximation, \( b(\xi) \) is the vector of the coefficients and \( H^T(\xi - \xi_j) \) is a vector containing the complete set of the monomials:

\[
H^T(\xi - \xi_j) = \left[1, (\xi_1 - \xi_{1j}), (\xi_2 - \xi_{2j}), (\xi_1 - \xi_{1j})^2, \ldots (\xi_1 - \xi_{1j})^n \right] 
\]

(4.4)

The following reproducing conditions are imposed:

\[
\sum_{j=1}^{N_s} C(\xi; \xi - \xi_j) \Phi_a(\xi - \xi_j) \xi_j^n \xi_{2j}^q = \xi_j^n \xi_{2j}^q 
\]

(4.5)

Substituting (4.3) into (4.5), \( b(\xi) \) is determined by solving the following equation:

\[
M(\xi) b(\xi) = H(0) 
\]

(4.6)

where \( M(\xi) \) is the moment matrix of the kernel function \( \Phi_a(\xi - \xi_j) \):

\[
M(\xi) = \sum_{j=1}^{N_s} H(\xi - \xi_j) H^T(\xi - \xi_j) \Phi_a(\xi - \xi_j) 
\]

(4.7)

To determine \( b(\xi) \), \( M(\xi) \) should be non-singular. Thus the support \( a \) of the kernel function \( \Phi_a(\xi - \xi_j) \) must be large enough to contain at least \( n \) non-co-linear or non-co-planer points.

The coefficients \( b(\xi) \) can be expressed as follows:

\[
b(\xi) = M^{-1}(\xi) H(0) 
\]

(4.8)
Substituting (4.2) into (4.1) in combination with (4.3) and (4.8), the approximation function can be described as follows:

\[ u^k(\xi) = \sum_{i=1}^{N_s} \Psi_i(\xi) d_i \]

\[ = \sum_{i=1}^{N_s} H^T(0)M^{-1}(\xi)H^T(\xi - \xi_i) d_i \]

(4.9)

In this work, the cubic spline function is employed as the kernel function:

\[ \Phi_a(\xi - \xi_i) = \prod_{i=1}^{n_{sd}} \frac{1}{a_i} \Phi_a \left( \frac{\xi_i - \xi_d}{a_i} \right) \]

(4.10)

\[ \tilde{\Phi}_a(z_{ik}) = \begin{cases} \frac{2}{3} - 4z_{ik}^2 + 4z_{ik}^3 & \text{for } 0 \leq |z_{ik}| \leq \frac{1}{2} \\ \frac{4}{3} - 4z_{ik} + 4z_{ik}^2 - \frac{4}{3}z_{ik}^3 & \text{for } \frac{1}{2} \leq |z_{ik}| \leq 1 \\ 0 & \text{otherwise} \end{cases} \]

(4.11)

where \( n_{sd} \) is the number of dimensionality. The cubic spline function is \( C^2 \) continuous providing higher smoothness than the \( C^0 \) or \( C^1 \) finite element approximation functions. Since the support of the RK basis function is the same as the support of the kernel function, the bandwidth of the resulting matrix of the linear system can be easily estimated. Furthermore, the degree of completeness and consistency of the monomial basis vector \( H(\xi - \xi_i) \) determines the order of convergence in function approximation and in solving PDEs. Similar to the finite element methods (FEM), the RK approximation yields algebraic convergence, since the approximation is based on local polynomials functions. For approximating a smooth function, the RK approximation provides higher accuracy than FEM, since the RK basis functions have higher smoothness than the FE shape functions. However, the RK basis functions do not possess Kronecker delta properties, i.e., \( \Psi_i(\xi_j) \neq \delta_{ij} \) such that the coefficients \( d_i \) are not the nodal values. Consequently this approximation scheme requires extra effort to determine the nodal values. Figure 4.1 illustrates the discretization and the
basis functions of a two-dimensional RK approximation, where the support of the kernel function can be rectangular or circular shapes.

Although the RK approximation reproduces polynomials, the approximation functions $\Psi_j(\xi)$ are not polynomials. For weak formulation, determining the coefficients requires domain integration, while the RK basis functions cannot be integrated exactly under the Gauss integration methods. To avoid domain integration issues, strong form based approaches have been considered as an alternative of the weak formulation. For solving differential equations with strong formulation, the methods require higher order smoothness in the approximation functions than those used in the weak formulation. Solving $n$-th order differential equations with strong formulation requires $n$-time differentiable approximation functions. Thus, the RK basis functions can be applied into the strong formulation naturally, since the approximation functions easily achieve high orders of smoothness by choosing appropriate kernel functions.

![Figure 4.1](image)

**Figure 4.1** (a) The RK discretization and compact support in two-dimension (b) the RK basis function
4.2 The Radial Basis Function (RBF) Approximation

Here, the Radial Basis function (RBF) is also introduced to approximate a random function. The construction of the RBF is based on the radius between the source point and the evaluation points. A few commonly used RBFs are listed below:

(1) Multi-quadrics (MQ):

\[ \Psi_i(\xi) = \left( r_i^2 + c^2 \right)^{\frac{3}{2}} \]  \hspace{1cm} (4.12)

(2) Gaussian:

\[ \Psi_i(\xi) = \begin{cases} \exp \left( - \frac{r_i^2}{c^2} \right) \\ \left( r_i^2 + c^2 \right)^{\frac{3}{2}} \exp \left( - \frac{r_i^2}{c^2} \right) \end{cases} \]  \hspace{1cm} (4.13)

(3) Thin plate splines:

\[ \Psi_i(\xi) = \begin{cases} r_i^{2n} \ln r_i \\ r_i^{2n-1} \end{cases} \]  \hspace{1cm} (4.14)

(4) Logarithmic:

\[ \Psi_i(\xi) = r_i^n \ln r_i \]  \hspace{1cm} (4.15)

For a 2-D case, \( \xi = (\xi_1, \xi_2) \), \( r_i = \sqrt{(\xi_1 - \xi_{1i})^2 + (\xi_2 - \xi_{2i})^2} \), and \( \xi_{ij} = (\xi_{1j}, \xi_{2j}) \). The constant \( c \) in (4.12) and (4.13) is called shape parameter. It controls the locality of the basis functions. For the MQ RBF of (4.12), the function is called reciprocal MQ RB function if \( n = 1 \), linear MQ RBF if \( n = 2 \), and cubic MQ RBF if \( n = 3 \), and so forth.

For a smooth function \( u(\xi) \), the approximation function denoted by \( u^h(\xi) \) is expressed as

\[ u^h(\xi) = \sum_{i=1}^{N_s} \Psi_i(\xi) d_i \]  \hspace{1cm} (4.16)

where \( N_s \) is the number of the source points (or basis functions). This method exhibits stable...
results when increasing the number of source points. The RBF approximation offers exponential convergence as has been discussed in the literature [31], and this property is responsible for its popularity in the field of approximation. Nevertheless, the RBF approximation suffers from ill-conditioning in large discrete systems. In (4.12) and (4.13), the selection of shape parameter $c$ affects the convergence and the conditions of the resulting matrices of linear systems. In general, a larger value of $c$ provides more accurate approximation for a smooth function, but it results in an ill-conditioned discrete system. As the discretization is refined, the condition worsens. Hence, an enhanced scheme named Localized Radial Basis Function (L-RBF) was proposed [38]. In this approach, the RK function is introduced as the localizing function such that the method inherits both the advantages of the RBF and RK approximations. L-RBF provides better conditioning than the global RBF approximation, while it also offers a higher rate of convergence than that of the RK approximation.

4.3 Accelerated RK and RB Approximations in the Random Space

As aforementioned, RK and RBF approximations are adopted for stochastic analyses, the concern now turns to the computational efficiency. For the RK approximation, the computational cost is mainly from the algorithm to construct the basis functions at the evaluation points. In order to derive the basis functions at each evaluation point, we need to follow the procedure from (4.7)–(4.9) to satisfy the reproducing conditions of monomials. Furthermore, as the order of the basis functions increases, the dimension of the moment matrix will expand such that the scheme requires more computation. On the other hand, for
the RBF approximation the main computational cost originates from solving the generalized coefficients. Since the support of the basis functions covers the entire domain, the attention then turns to solving a linear system of equations involving full matrices. As the dimensionality increases, the cost for solving the generalized coefficients will increase exponentially. Such phenomenon is termed “curse of dimensionality”. In this section, new algorithms will be presented to enhance the efficiency of the RK and RBF approximations.

4.3.1 Accelerated RK Approximation in the Uniform Domain

In stochastic analysis, the domain of the random variables is typically rectangular. Consequently the approximation of the random variables can be constructed by tensor product of approximation in each dimension. Consider here a RK approximation in one-dimension with an equally spaced discretization and constant support size. With this discretization, the approximation function in the region away from the boundaries is periodic. As shown in Figure 4.2, considering two points $x_{i+\alpha}$ and $x_{i+1+\alpha}$, which have the same relative location to their neighboring nodes, the approximation functions can be written in the following expression:

$$
f^{a}(x_{i+\alpha}) = \ldots + \Psi((\alpha-1)h)a_{i-1} + \Psi(\alpha h)a_{i} + \Psi((1-\alpha)h)a_{i+1} + \ldots$$

$$
f^{a}(x_{i+1+\alpha}) = \ldots + \Psi((\alpha-1)h)a_{i} + \Psi(\alpha h)a_{i+1} + \Psi((1-\alpha)h)a_{i+2} + \ldots \quad (4.17)$$

For points close to the boundaries, the approximation does not follow the same characteristics. This occurs because these points are not covered by the same number of supports of nodes as those of the interior points. To enforce the periodical properties in the RK shape functions throughout the entire domain, one can add the virtual nodes outside of the boundaries as shown in Figure 4.3. The nodal values of the virtual nodes are then determined by taking the following finite element extrapolation scheme:

$$
f^{a}_{n+1} = \ldots + N_{n}(x_{n+1})f_{n} + N_{n-1}(x_{n+1})f_{n-1} + \ldots \quad (4.18)$$

43
where $N(x)$ is the finite element (FE) shape function. For linear extrapolation case,

\[ f_{n} = f_{n-1} \]
\[ f_{n+1} = 2f_{n} - f_{n-1} \]

\[ f_{n+1} = 2f_{0} - f_{1} \]  

(4.19)

The number of virtual nodes is determined by the size of support. When the normalized support size is less than 2, only 1 extra node is required for each of the boundaries. This approach avoids the need to construct the basis functions for every nodes.

### 4.3.2 Computational Reduction for Multi-dimensional Problems

Let the approximation of a function in multi-dimension be expressed in the following general form:

\[ f^a(x_1, x_2, \ldots, x_d) = \sum_{i=1}^{N_1 \times N_2 \times N_d} \Phi_i(x_1, x_2, \ldots, x_d) \hat{a}_i \]  

(4.20)

To construct the linear system of equations and determine the corresponding coefficients, this formulation requires solving a large linear system as shown in the following equation:

\[ \begin{align*}
    a_1 & = \frac{1}{2} a_0 + \frac{1}{2} a_2 \\
    a_i & = a_{i-2} + a_{i+2} \\
    a_{n+1} & = \frac{1}{2} a_n + \frac{1}{2} a_{n-2} \\
    a_n & = 0
\end{align*} \]
\[ \Psi \hat{a}_i = f \]  

(4. 21)

If the collocation points coincide with the source points, the terms in the above equation are:

\[
\Psi = \begin{bmatrix}
\Psi_1 (\xi^1) & \cdots & \Psi_{N_\xi} (\xi^1) \\
\vdots & \ddots & \vdots \\
\Psi_1 (\xi^{N_\xi}) & \cdots & \Psi_{N_\xi} (\xi^{N_\xi})
\end{bmatrix}, \\
\mathbf{f} = \begin{bmatrix}
f(\xi^1) \\
\vdots \\
f(\xi^{N_\xi})
\end{bmatrix}, \\
\hat{\mathbf{a}} = \begin{bmatrix}
a_1 \\
\vdots \\
a_{N_\xi}
\end{bmatrix}
\]  

(4. 22)

Using the same degrees of freedom \( N \) in each dimension, the corresponding dimensions of the matrix \( \Psi \) are:

\[ N_c \times N_c = N^d \times N^d \]  

(4. 23)

This algorithm can be viewed as a Full Transformation (FT) between the generalized coefficients and the nodal coefficients. Since the algorithm requires extremely high computation and storage for solving the coefficients, alternative solving algorithms are required. By utilizing the stochastic characteristics, the approximated function can be decomposed as:

\[ f^a (\xi) = F_1 (\xi_1) \otimes F_2 (\xi_2) \otimes \cdots \otimes F_d (\xi_d) \]  

(4. 24)

where \( F_i (\xi_i) \) is the \( k \)-th dimensional function, \( d \) is the dimensionality and \( \otimes \) denotes the tensor product operator. Let the approximation be expressed as:

\[ f^a (\xi_1, \xi_2, \ldots, \xi_d) = \sum_{i_1=1}^{N_1} \cdots \sum_{i_d=1}^{N_d} \sum_{i_k=1}^{N_k} \Psi_{a_k}^k (\xi_1) \Psi_{b_1}^1 (\xi_2) \cdots \Psi_{b_d}^d (\xi_d) a_{i_1\cdots i_d} \]  

(4. 25)

where \( \Psi_{a_k}^k (\xi_k) \) and \( N_k \) are the basis functions and the number of degrees of freedom in the \( k \)-th dimension respectively, and \( a_{i_1\cdots i_d} \) are the generalized coefficients to be determined.

Using Galerkin procedures, assume that there exists a set of test functions \( P_{j_k}^k (\xi_k) \) such that it satisfies the following properties:

\[ (P_{j_k}^k, \Psi_{a_k}^k) = \int_{\Omega_k} P_{j_k}^k (\xi_k) \Psi_{a_k}^k (\xi_k) d\xi_k = \delta_{a_k j_k} \]  

(4. 26)

where \( (\cdot, \cdot) \) denotes the integration operator. The generalized coefficients are then derived as shown below:
To construct \( P^k_i(\xi_k) \), take discrete form for (4.26)

\[
\left( P^k_i, \Psi^k_j \right) = \sum_{p=1}^{N_k} P^k_i(\xi^p_k) \Psi^k_j(\xi^p_k) \equiv p^k_{i,p} \Psi^k_j = \delta_{i,j}
\]

where \( \xi^p_k \) are the collocation points in the \( k \)-th dimension, and \( \Psi^k_j \equiv \Psi^k_j(\xi^p_k) \). Here Einstein’s summation convention is used for each tensorial term with repeated dummy index.

Furthermore, enforcing the collocation points to coincide with the discrete points associated with the basis functions \( \Psi^k_i(\xi_k) \) (source points), the test functions \( P^k_i(\xi_k) \) is obtained:

\[
P^k_i = \left( \Psi^k_i \right)^{-1}
\]

or in matrix form:

\[
P^k = \left( \Psi^k \right)^{-1}
\]

where \( P^k \) is termed the directional transformation matrix. The generalized coefficients then can be solved as:

\[
a_{i_{12}\ldots ij} = P^1_{i_{1} p_{1}} P^2_{i_{2} p_{2}} \ldots P^d_{i_{d} p_{d}} f_{p_{1} p_{2} \ldots p_{d}}
\]

We call this algorithm the Directional Transformation (DT) method. For the approximation functions with compact support, \( \Psi^k \) is banded, but the inverse \( P^k \) is not necessarily banded. For the sake of improving the efficiency, the solution process is decomposed into \( d \) steps:

\[
\Psi^1_{i_{1} p_{1}} F^1_{i_{1} p_{2} \ldots p_{d}} = f_{p_{1} p_{2} \ldots p_{d}}
\]

\[
\Psi^2_{i_{2} p_{2}} F^2_{i_{2} p_{3} \ldots p_{d}} = F^1_{i_{1} p_{2} \ldots p_{d}}
\]

\[
\vdots
\]

\[
\Psi^d_{i_{d} p_{d}} a_{i_{d-1} \ldots ij} = F^{d-1}_{i_{d-1} p_{d}}
\]

To determine the coefficients \( a_{i_{12}\ldots ij} \) and \( F^k_{i_{12}\ldots i_{d} p_{1} \ldots p_{d}} \), simply repeat the Gaussian elimination algorithm \( \left(N^1 \times N^2 \times \ldots N^d \right)/N^k \) times for each step. We call this algorithm
Decomposed Gaussian Elimination (DGE).

To compare the performance of the proposed approaches with the conventional formulation, the operation counts for proposed approximations are estimated. Adopting Gaussian Elimination along with Backward Substitution to solve the linear systems and considering the same degrees of freedom $N$ in each dimension, the operation counts for a full matrix system with different algorithms are presented subsequently:

**Full Transformation (FT):**

\[
\text{M/D: } \left( \frac{N^{3d}}{3} + N^{2d} - \frac{N^d}{3} \right) \quad (4.33)
\]

\[
\text{A/S: } \left( \frac{N^{3d}}{3} + \frac{N^{2d}}{2} - \frac{5N^d}{6} \right) \quad (4.34)
\]

where the M/D and A/S stand for multiplication/division and addition/subtraction operations, respectively.

**Directional Transformation (DT) (for $d \geq 2$):**

\[
\text{M/D: } dN^{d+1} + d \left( \frac{N^4}{3} + N^3 - \frac{N^2}{3} \right) \quad (4.35)
\]

\[
\text{A/S: } dN^{d+1} + d \left( \frac{N^4}{3} + \frac{N^3}{2} - \frac{5N^2}{6} \right) \quad (4.36)
\]

In (4.35) and (4.36), the first terms are the operation counts for tensor operation in (4.31), while the second terms result from solving the inverse matrix of one-dimensional cases in (4.30).

**Decomposed Gaussian Elimination (DGE):**

\[
\text{M/D: } d \left( \frac{N^{d+2}}{3} + \frac{N^{d+1}}{3} - \frac{N^d}{3} \right) \quad (4.37)
\]

\[
\text{A/S: } d \left( \frac{N^{d+2}}{3} + \frac{N^{d+1}}{2} - \frac{5N^d}{6} \right) \quad (4.38)
\]

As can be seen in (4.33)–(4.38), the highest order of operation counts for DT and DGE are
only \( d+1 \) and \( d+2 \) respectively, while for FT the highest order is \( 3d \). As \( d \) increases, FT requires higher computation than the proposed algorithms. The comparisons of the operation counts for 2-D and 3-D problems with different algorithms are listed in Table 4.1, which demonstrates the advantages of the proposed approximation schemes.

### Table 4.1 Operation counts for solving full matrices (global approximation)

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>M/D</th>
<th>A/S</th>
<th>Normalized M/D</th>
<th>Normalized A/S</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>2-dimensional problems (N=100)</strong></td>
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<tr>
<td>FT</td>
<td>333,433,330,000</td>
<td>333,383,325,000</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>DT</td>
<td>70,660,000</td>
<td>69,650,000</td>
<td>0.000211916</td>
<td>0.0002089</td>
</tr>
<tr>
<td>DGE</td>
<td>68,660,000</td>
<td>67,650,000</td>
<td>0.000205918</td>
<td>0.0002029</td>
</tr>
<tr>
<td><strong>3-dimensional problems (N=100)</strong></td>
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<tr>
<td>FT</td>
<td>333,334,333,333,000,000</td>
<td>333,333,833,332,500,000</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>DT</td>
<td>402,990,000</td>
<td>401,475,000</td>
<td>1.20897E-09</td>
<td>1.204E-09</td>
</tr>
<tr>
<td>DGE</td>
<td>10,299,000,000</td>
<td>10,147,500,000</td>
<td>3.08969E-08</td>
<td>3.044E-08</td>
</tr>
</tbody>
</table>

Furthermore, the required storage for solving the generalized coefficients is as follows:

**Full Transformation (FT):**

\[
\text{Required storage} = N^{2d} + 2N^d \quad (4. 39)
\]

**Directional Transformation (DT):**

\[
\text{Required storage} = 2N^d + 2dN^2 \quad (4. 40)
\]

**Decomposed Gaussian Elimination (DGE):**

\[
\text{Required storage} = 2N^d + dN^2 \quad (4. 41)
\]

Clearly FT requires the largest storage in comparison to the proposed algorithms. The comparison shows that the proposed DT and DGE algorithms are better choices when \( d > 2 \).

For approximations with locality, i.e. the RK approximation, DGE and FT are further compared. Since \( P^d \) are not guaranteed to be band matrices, solving the coefficients by DT
still requires calculation through all the degrees of freedom. For DGE, the banded structure in \( \Psi^k \) helps reduce the computational cost. For using local approximations to solve a system, let the bandwidth of the matrix in the 1-D cases be \((2w_1-1)\), where \(w_1\) is the half bandwidth of one dimensional case, the operation counts for DGE are:

\[
M/D: \left[ d(w_1^2 + w_1 - 1)N^d - d\left(\frac{2}{3}w_1^3 - \frac{2}{3}w_1\right)N^{d-1}\right] \quad (4.42)
\]

\[
A/S: \left[ d(w_1^2 - 1)N^d - d\left(\frac{2}{3}w_1^3 - \frac{1}{2}w_1^2 - \frac{1}{6}w_1\right)N^{d-1}\right] \quad (4.43)
\]

For FT, we consider uniform bandwidth for simplicity, and the operation counts are:

\[
M/D: \left[ (w_d^2 + w_d - 1)N^d - \frac{2}{3}w_d^3 + \frac{2}{3}w_d\right] \quad (4.44)
\]

\[
A/S: \left[ (w_d^2 - 1)N^d - \frac{2}{3}w_d^3 + \frac{1}{2}w_d^2 + \frac{1}{6}w_d\right] \quad (4.45)
\]

where \((2w_d-1)\) is the bandwidth for multi-dimensional problems such that:

\[
w_d \approx \frac{(2w_1-1)^d + 1}{2} \quad (4.46)
\]

where \(w_1\) is the half-bandwidth in one dimension.

Using the RK approximation, the value of \(w_1\) is determined by the normalized support size. For normalized support size ranges between 1 and 2, \(w_1=2\); between 2 and 3, \(w_1=3\); between 3 and 4, \(w_1=4\); and etc. From (4.46), we have

\[
w_d >> d(w_1^2 + w_1 - 1) \quad (4.47)
\]

Thus as the dimensionality increases, the difference between FT and DGE becomes more pronounced. Table 4.2 validates the comparisons of the operation counts for 2-D and 3-D problems.
Table 4.2 Operation counts for solving banded matrices (local approximation)

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>( w_1 )</th>
<th>M/D</th>
<th>A/S</th>
<th>Normalized M/D</th>
<th>Normalized A/S</th>
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<tbody>
<tr>
<td><strong>2-dimensional problems (N=100)</strong></td>
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<tr>
<td>FT ( w_1=2 ) (Supp=1.5)</td>
<td>FT ( w_1=3 ) (Supp=2.5)</td>
<td>FT ( w_1=2 ) (Supp=1.5)</td>
<td>FT ( w_1=3 ) (Supp=2.5)</td>
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Here the accelerated RK and RBF formulations presented in Section 4.3 are used in the computation for comparison. The $L_2$ error norms are calculated for comparison of the convergence, as shown in Figure 4.4. The RBF approximation shown in Figure 4.4 demonstrates an exponential convergence, while the RK approximation yields algebraic convergence rate. The comparison of FT and DT methods for the RBF approximation shown in Table 4.3 demonstrates the significant efficiency and memory advantages in the DT approach.

![Figure 4.4 Comparison of L2 error norm between two different schemes](image)

Table 4.3 CPU time for solving generalized coefficients

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The RBF approximation with Smolyak algorithm is also investigated. Here, Multi-quadrics radial basis function is introduced for approximation in 1-D, and the
collocation points are selected to coincide with the source points. The shape parameter $c=0.4$ is selected, and the total level of algorithm $N$ is studied below. At the $i$-th sub-level, the number of the collocation points is $(2^{i-1}+1)$ as $i>1$, and the number of collocation points is 1 for $i=1$. With $q=N+1$, the expression is written as follows:

$$f^a = \sum_{N=1}^{N+1} (-1)^{N-H} \left( \frac{1}{N+1-|H|} \right) \sum_{i} \sum_{j} \Psi^i_j(x) \Psi^j_i(y) a^{ij}_{ij}$$

$$\equiv A(N+1,2)(f)$$  (4.49)

Solve $a^{ij}_{ij}$ independently for each term of the linear combination $\Psi^i_j \otimes \Psi^j_i$. Then the approximation function of $f(x,y)$ can be obtained up to order $q=N+1$.

![Figure 4.5 Error norm vs. number of nodes](image)

**Figure 4.5 Error norm vs. number of nodes**

![Figure 4.6 The layout of the nodes as N=6](image)

(a) Somlyak algorithm as $q=7$ (145 nodes)  
(b) full set (1,089 nodes)

**Figure 4.6 The layout of the nodes as $N=6$**
The numerical performance is illustrated in Figure 4.5, where the ordinate is the $L_2$ error norm for estimating the accuracy of the approximation, while the abscissa is the number of nodes. The figure compares the cases of full set of nodes with the reduced sets by using the Smolyak algorithm. As the figure shows, for the accuracy of the Smolyak algorithm and the use of full sets of nodes, the Smolyak algorithm shows better efficiency than the use of all nodes. For the case with $N=6$ and $q=7$, the total nodes required by employing Smolyak algorithm are only 145, whereas the full set of nodes is 1,089. The layout of the nodes for Smolyak algorithm and the full set are both shown in Figure 4.6.

### 4.4.2 The Kraichnan-Orszag Three-mode Problem

This problem was first studied by Kraichnan using large Gaussian samples. Orszag and Bissonnette [25] showed that polynomial chaos failed to converge for this problem. Wan and Karniadakis [26] used multi-element generalized polynomial chaos (ME-gPC) to solve this problem by decomposing the random space into several sub-domains.

Consider the nonlinear three-dimensional stochastic ODE system:

$$
\frac{dy_1}{dt} = y_1 y_3, \quad \frac{dy_2}{dt} = -y_2 y_3, \quad \frac{dy_3}{dt} = -y_1^2 + y_2^2 \tag{4. 50}
$$

where $y_1$, $y_2$ and $y_3$ are functions of $t$ subjected to stochastic initial conditions:

$$
y_1(t = 0) = 1, \quad y_2(t = 0) = 0.1 \xi, \quad y_3(t = 0) = 0 \tag{4. 51}
$$

where $\xi$ is a uniform random variable within the range [-1, 1].

Four numerical approximation methods are adopted for comparison: the RBF approximation, the RK approximation, the generalized polynomial chaos (gPC) and the multi-element generalized polynomial chaos (ME-gPC). In this example, 4-th order Runge-Kutta methods are adopted to solve the deterministic ODE problem. For the first two approaches, the collocation method is used to determine the coefficients, while Galerkin
approximation is adopted for the last two methods. Figure 4.7 shows the comparison of the four different approximation methods, where the Monte Carlo simulation (MCS) is taken as the referenced solution. The results show that the RK and RBF approximations have better accuracy than gPC and ME-gPC. Comparing the average of $y_1(t)$, all four approximation schemes agree well with MCS. While, for standard deviation, the solution of gPC deviates from the reference solution as time increases. Figure 4.7(d) clearly illustrates why gPC fails to converge. As can been seen, the gPC approximation yields numerical oscillation. The oscillation is due to the occurrence of discontinuity at $\xi=0$. gPC constitutes a p-type refinement, where the increase of degrees of freedom (DOF) activates higher order polynomial basis functions which yields the Gibbs phenomenon. Hence, approximation by high order global polynomial functions is typically oscillatory. On the other hand, h-type refinement is employed in the RBF and RK approximations. Furthermore, the RK approximation is a local approximation which is well-conditioned during model refinement. The ME-gPC method yields a slight improvement over gPC, but is still substantially less accurate than the RK and RBF approximations.
Figure 4.7 Comparisons among different approximation schemes
4.4.3 A Cantilever Subjected to a Uniform Distributed Load

This example considers a cantilever beam subjected to a uniform distributed load \( q \) as shown in Figure 4.8. Assume the bending rigidity can be decomposed into a deterministic part \( \bar{w}(x) \) and a stochastic part \( \alpha(x, \theta) \), where \( \bar{w}(x) \) is the mean bending rigidity and \( \alpha(x, \theta) \) is the deviation of the bending rigidity represented by Karhunen-Loève (K-L) expansion:

\[
\alpha(x, \theta) = \sum_{n=0}^{\infty} \sqrt{\lambda_n} \xi_n(\theta) f_n(x)
\]  

(4.52)

where \( \xi_n(\theta) \) are independent random events with Gaussian probability distribution, and \( \lambda_n \) and \( f_n(x) \) are eigenvalues and eigenfunctions that are determined by the following covariance function:

\[
C_{\alpha\alpha}(x_1, x_2) = \sigma^2 e^{-|x_1 - x_2|^b}
\]  

(4.53)

where \( \sigma \) is the standard deviation of the bending rigidity and \( b=1 \) is the correlation length defining the relationship of \( \alpha(x, \theta) \) between any two points \( x_1 \) and \( x_2 \). In this problem, 2-term K-L expansion is adopted, and the random numbers are generated in the following domain:

\[
\Omega_\xi \in [-1.75,1.75] \times [-1.75,1.75]
\]  

(4.54)

\[ q(x) = 1, \ L = 1, \ \bar{w}(x) = 1, \]

Figure 4.8 A cantilever beam subjected to a uniform distributed load

Figure 4.9 illustrates the comparison of the numerical results generated by the RBF approximation, the RK approximation, Homogeneous Chaos, as well as the Monte Carlo reference solution. For the RBF and RK approximations, 4x4 and 5x5 source points for each method are considered. The RBF approximation employs a linear MQ function with shape
parameter $c=10.0$, and the RK approximation introduces quadratic basis with normalized support size $=2.5$. The numerical results show that the RBF and RK approximations perform better than the homogeneous chaos approach. As the standard deviation of the bending rigidity increases, the 4-th order homogeneous chaos shows numerical oscillations. The oscillations in the homogeneous chaos approach stem from the inconsistency between the Gaussian probability distribution used in the homogeneous chaos formulation to maintain the orthogonality with respect to the stochastic process and the truncated Gaussian probability distribution used in describing the uncertainty in the bending rigidity of the beam.

![Graph](image)

(a) Average of tip deflection vs. standard deviation of bending rigidity

![Graph](image)

(b) Standard deviation of tip deflection vs. standard deviation of bending rigidity

Figure 4.9 The comparison for the average and standard deviation of the beam tip deflection among different numerical methods.
Chapter 5

Crack Modeling Using Enriched RKPM

The singularities and discontinuities in the crack behavior cannot be effectively modeled by the conventional polynomial based approximation methods. Extrinsic enrichment methods under the framework of mesh-free methods have been introduced to model the crack problems. Three different extrinsic enrichment approaches will be discussed in this chapter: the first is the singular enrichment for the near-tip field used in linear elastic fracture mechanics (LEFM), the second is the cohesive zone model enrichment as a means to regularize the singularity occurring in LEFM and the third enrichment scheme is the proposed approach which utilizes the visibility criterion while preserving the Partition of Unity (POU) property for the enriched mesh-free approximation function to ensure mass conservation in the discrete system. The proposed enrichment method is then verified by conducting several benchmark fracture problems.

5.1 Formulation of Extrinsically Enriched RKPM

An extrinsically enriched RKPM formulation has been introduced to model the crack surface for fracture mechanics based numerical simulation. In the literature, the extrinsic enrichment methods are expressed in the following form [40-44]:

58
\[ u^b(x) = \sum_{i \in N} \Psi_i(x) d_i + \sum_{j \in N_{cut}} H(x) \Psi_j(x) a_j + \sum_{k \in N_{tip}} F_k(x) \Psi_k(x) b_k \]  \hspace{1cm} (5.1)

where \( \Psi_i(x) \) is the conventional RK shape function possessing reproducibility of polynomials as discussed in Chapter 4, \( N \) is the total node sets, \( N_{cut} \) is the number of the enriched nodes whose supports are cut through by the crack surface and \( N_{tip} \) is the number of the near-tip enriched nodes. The enrichment function \( H(x) \) is expressed in the following form:

\[ H(x) = \begin{cases} 1 & y > 0 \\ -1 & y < 0 \end{cases} \]  \hspace{1cm} (5.2)

where \( y \) is the local coordinate system aligned with the crack surface as described in Figure 5.1.

![Figure 5.1 A crack in a domain with the mesh-free approximation](image)

For linear elastic fracture mechanics (LEFM), singular tip enrichment functions [40-41] are employed:

\[ \{ F_i(x) \} = F(r, \theta) = \{ \sqrt{r} \sin \left( \frac{\theta}{2} \right), \sqrt{r} \cos \left( \frac{\theta}{2} \right), \sqrt{r} \sin \left( \frac{3\theta}{2} \right), \sqrt{r} \cos \left( \frac{3\theta}{2} \right) \} \]  \hspace{1cm} (5.3)

For the cohesive zone model, the following enrichment functions [43] are considered:

\[ \{ F_i(x) \} = F(r, \theta) = \left\{ r \sin \left( \frac{\theta}{2} \right), r^{\frac{3}{2}} \sin \left( \frac{\theta}{2} \right), r^2 \sin \left( \frac{\theta}{2} \right) \right\} \]  \hspace{1cm} (5.4)

Note that the un-enriched finite dimensional RK shape functions satisfy the condition of
Partition of Unity (POU) since the reproducing conditions include the reproducibility of a constant base:

$$\sum_{j=1}^{NP} \Psi_j(x) = 1 \quad (5.5)$$

This property is required for constructing the approximation function to represent the enriched displacement field [40-42]. This work exploits the POU property into the enriched mesh-free methods or finite element methods [45], which allows enrichment functions to be incorporated into a finite dimensional approximation while preserving POU property. Note that the enriched approximation methods do not preserve POU property for the enriched near-tip field unless a special treatment is introduced. Here a different enrichment scheme is proposed based on the visibility criterion and the preservation of POU property for the enriched near-tip displacement field:

$$u^b = \sum_{l \in N \cap N_{cut} \cup N_{tip}} \Psi_l(x) d_l + \sum_{j \in N_{cut}, i=1,2} H_i(x) \Psi_j(x) a_{ij} + \sum_{k \in N_{tip}, i=1,2} f_i(x) \Psi_{ik}(x) b_{ik} \equiv \sum_l \Psi_l(x) \bar{d}_l \quad (5.6)$$

To preserve the POU property, we require

$$\sum_l \bar{\Psi}_l(x) = \sum_{l \in N \cap N_{cut} \cup N_{tip}} \Psi_l(x) + \sum_{j \in N_{cut}, i=1,2} H_i(x) \Psi_j(x) + \sum_{k \in N_{tip}, i=1,2} f_i(x) \Psi_{ik}(x) = 1 \quad (5.7)$$

Note that the regular nodal set with smooth RK approximation has excluded the enriched nodes $N_{cut}$ and $N_{tip}$, hence the POU property holds as the enrichment functions $H_i(x)$ and $f_i(x)$ satisfy the following conditions:

$$H_1(x) + H_2(x) = 1 \quad (5.8)$$

$$f_1(x) + f_2(x) = 1 \quad (5.9)$$

Since the standard RKPM also satisfies the POU property, (5.7) holds as long as the
enrichment functions satisfy the conditions of (5.8) and (5.9). Here the heaviside functions are introduced for the off-tip enrichment which provides the discontinuity for the displacement field:

\[ H_1(x) = \begin{cases} 1 & \text{if } y > 0 \\ 0 & \text{if } y < 0 \end{cases} \quad (5.10) \]

\[ H_2(x) = 1 - H_1(x) \quad (5.11) \]

The graphical illustration of the enriched shape function is shown in Figure 5.2. The original RK shape function of node \( J \) is dissected by the crack surface to represent the discontinuity on the crack surface. The original shape functions are equivalent to the combination of two separated shape functions. Hence, the POU property is still preserved.

$$\begin{align*}
H_1(x) &= \begin{cases} 1 & \text{if } y > 0 \\ 0 & \text{if } y < 0 \end{cases} \\
H_2(x) &= 1 - H_1(x)
\end{align*}$$

**Figure 5.2 The graphical illustration for the heaviside enrichment function**

Similarly, the near-tip field enrichment function \( f_i(x) \) to be constructed follows the same concept. As illustrated in Figure 5.3, the un-enriched shape function is separated into two independent functions along the connected line of the node and crack tip and the first enrichment function \( f_i(x) \) is built by introducing visibility criterion [48-49] such that the discontinuity stops at the crack tip:

\[
\begin{align*}
1 & \quad \frac{\theta_0}{2} \leq \theta \leq \pi \\
\sin(\theta - \theta_0 + \pi) & \quad -(\pi - \theta_0) \leq \theta < \theta_0 - \frac{1}{2} \pi \\
0 & \quad -\pi \leq \theta < -\pi - \theta_0
\end{cases}
\]

For \( \theta_0 > 0 \),

\[
f_i(x) = \begin{cases} 1 & \frac{\theta_0}{2} \leq \theta \leq \pi \\
\sin(\theta - \theta_0 + \pi) & -(\pi - \theta_0) \leq \theta < \theta_0 - \frac{1}{2} \pi \\
0 & -\pi \leq \theta < -(\pi - \theta_0)
\end{cases}
\]

(5.12)
Here, as illustrated in Figure 5.3, $\theta_0$ is the angle between the $x$-axis and the connected line of the crack tip and the enriched node and $\theta$ is the angle between $x$-axis and the radius of the evaluation point. The enrichment function $f_2(x)$ is defined to ensure that the shape functions satisfy the condition of POU, that is

$$f_2(x) = 1 - f_1(x)$$  \hspace{1cm} (5.14)

Figure 5.3 The illustration of crack tip enrichment functions

Note that the enriched shape functions only provide discontinuity across the crack surface but no singularity is introduced in the enrichment function. Here the POU concept for the near-tip enrichment is different from the standard X-FEM, where the POU property is required for constructing the approximation function to represent the enriched displacement field. The proposed enrichment method is to preserve the POU property, which guarantees the conservation of mass of the discrete system for modeling the dynamic fracture problems. The numerical complexity is reduced in the proposed method for the changing discretization when cracks propagate. On the other hand, the conventional tip-enrichment schemes, such as
asymptotic enrichment methods in (5.3) and (5.4), conventional visibility, or diffraction criteria, do not preserve the conservation of the mass. More details will be discussed in the following section.

5.2 An Explicit Time Integration Method for Crack Propagation

5.2.1 A Lumped Mass Scheme

In this section, the central difference method with lumped mass scheme is employed for the time integration of dynamic crack propagation. The lumped mass matrix is constructed by summing up the mass components of each row of the consistent mass matrix. The component $m_{ij}$ of the consistent mass matrix is firstly obtained by integrating the product the two shape functions $I$ and $J$:

$$m_{ij} = \int_{\Omega} \rho \overline{\Phi}_I(x) \overline{\Phi}_J(x) \, d\Omega$$  \hspace{1cm} (5.15)

Here, we consider the enriched approximation method which preserves the POU property after enriching as defined in (5.7). Note that $\overline{\Phi}_I(x)$ includes the enriched shape functions as shown in (5.6). The lumped mass of node $I$ can then be obtained by summing up the components of the $I$-th row:

$$m_{II} = \sum_j m_{ij} = \sum_j \int_{\Omega} \rho \overline{\Phi}_I(x) \overline{\Phi}_J(x) \, d\Omega = \int_{\Omega} \rho \overline{\Phi}_I(x) \sum_j \overline{\Phi}_J(x) \, d\Omega$$  \hspace{1cm} (5.16)

Since the enriched approximation preserves the POU property as shown in (5.7), (5.16) can be rewritten as

$$m_{II} = \int_{\Omega} \rho \overline{\Phi}_I(x) \, d\Omega$$  \hspace{1cm} (5.17)
This approach is the same as the standard lumped mass method, in which the mass matrix is diagonal.

### 5.2.2 Update of the Nodal Coefficients of Additional Bases due to Crack Propagation

For modeling the dynamic crack propagation, a critical step is to reconstruct the discrete linear momentum equation as the crack propagates. At time $t_n$, the equation of linear momentum can be expressed as:

$$
\mathbf{M}_n \mathbf{a}_n = \mathbf{f}^\text{ext}_n - \mathbf{f}^\text{int}_n - \mathbf{f}^\text{damp}_n 
$$

(5.18)

where $\mathbf{f}^\text{ext}_n$ is the external force, $\mathbf{f}^\text{int}_n$ is the internal force and $\mathbf{f}^\text{damp}_n$ is the damping force, $\mathbf{a}_n$ is the acceleration vector at time $t_n$. Denote $\mathbf{v}_n$ as the velocity vector:

$$
\mathbf{a}_n = \frac{d^2 \mathbf{d}_n}{dt^2}, \quad \mathbf{v}_n = \frac{d \mathbf{d}_n}{dt}
$$

(5.19)

When the crack propagates, the approximation bases change in respond to the newly formed crack surface. To determine the coefficients of the new bases before the time advances to the next step, the conservation laws of kinetic energy and linear momentum are imposed upon each enriched node $I$, where the predictors of the enriched nodal velocities at the next time step $t_{n+1}$ are denoted as $\mathbf{\tilde{v}}_{la}^{n+1}$ and $\mathbf{\tilde{v}}_{lb}^{n+1}$, and the predictors of the nodal masses are $\mathbf{\tilde{m}}_{la}^{n+1}$ and $\mathbf{\tilde{m}}_{lb}^{n+1}$. The conservation laws of linear momentum and kinetic energy can then be expressed as:

$$
m_{la}^n \mathbf{v}_{la}^n + m_{lb}^n \mathbf{v}_{lb}^n = \mathbf{\tilde{m}}_{la}^{n+1} \mathbf{\tilde{v}}_{la}^{n+1} + \mathbf{\tilde{m}}_{lb}^{n+1} \mathbf{\tilde{v}}_{lb}^{n+1}
$$

(5.20)

$$
\frac{1}{2} m_{la}^n (\mathbf{v}_{la}^n)^2 + \frac{1}{2} m_{lb}^n (\mathbf{v}_{lb}^n)^2 = \frac{1}{2} \mathbf{\tilde{m}}_{la}^{n+1} (\mathbf{\tilde{v}}_{la}^{n+1})^2 + \frac{1}{2} \mathbf{\tilde{m}}_{lb}^{n+1} (\mathbf{\tilde{v}}_{lb}^{n+1})^2
$$

(5.21)

where a quantity with a superposed symbol "\~" denotes the predictor of the quantity at time $t_{n+1}$ referenced at the configuration of time $t_n$. The subscripts $a$ and $b$ represent the quantities...
related to two shape functions separated by the crack surface, which are corresponding to the nodal coefficients $b_{1K}$ and $b_{2K}$ in (5.6), respectively, e.g., for nodes enriched by the near-tip enrichment functions:

\[ m_{1n}^n = \int_{\Omega} \rho f_n^1(x) \Psi_I(x) \, d\Omega, \quad m_{2n}^n = \int_{\Omega} \rho f_n^2(x) \Psi_I(x) \, d\Omega \]  
(5.22)

\[ \tilde{m}_{1n+1}^n = \int_{\Omega} \rho f_{1n+1}^n(x) \Psi_I(x) \, d\Omega, \quad \tilde{m}_{2n}^n = \int_{\Omega} \rho f_{2n+1}^n(x) \Psi_I(x) \, d\Omega \]  
(5.23)

Note that $m_{1n}^n + m_{2n}^n = \tilde{m}_{1n+1}^n + \tilde{m}_{2n}^n = m_{\eta n}$, since the conditions of POU are preserved:

\[ f_n^1(x) + f_n^2(x) = f_{1n+1}^n(x) + f_{2n+1}^n(x) = 1 \]  
(5.24)

As illustrated in Figure 5.4, when a crack propagates, the near-tip enrichment functions will be advanced to the next time step $t_{n+1}$. The support is truncated by the crack with the visibility criterion. The mass at time $t_n$ and $t_{n+1}$ are the same due to the preservation of partition of unity, even if the discretization is changed. The linear momentum and kinetic energy of the are also conservative since the two conditions are imposed as shown in (5.20) and (5.21) when the discretization changes.
The predictors of the nodal velocities $\tilde{v}_{la}^{n+1}$ and $\tilde{v}_{lb}^{n+1}$ at time $t_{n+1}$ can be determined by solving (5.20) and (5.21):

$$\tilde{v}_{la}^{n+1} = \frac{m_{la}^n v_{la}^n + m_{lb}^n v_{lb}^n}{m_{la}^n + m_{lb}^n} + \sqrt{m_{la}^n m_{lb}^n} \frac{m_{la}^{n+1}}{m_{la}^n} (v_{la}^n - v_{lb}^n)$$  \hspace{1cm} (5.25)

$$\tilde{v}_{lb}^{n+1} = \frac{m_{lb}^n v_{lb}^n + m_{la}^n v_{la}^n}{m_{la}^n + m_{lb}^n} - \sqrt{m_{la}^n m_{lb}^n} \frac{m_{lb}^{n+1}}{m_{lb}^n} (v_{lb}^n - v_{la}^n)$$  \hspace{1cm} (5.26)

The predictors of the nodal accelerations at time $t_{n+1}$ are then obtained by re-evaluating the forces at time $t_{n+1}$:

$$\tilde{a}_{la}^{n+1} = \frac{1}{m_{la}^{n+1}} \left( (\tilde{v}_{la}^{n+1})^{\text{ext}} - (\tilde{f}_{la}^{n+1})^{\text{int}} - (\tilde{f}_{la}^{n+1})^{\text{damp}} \right)$$  \hspace{1cm} (5.27)

$$\tilde{a}_{lb}^{n+1} = \frac{1}{m_{lb}^{n+1}} \left( (\tilde{v}_{lb}^{n+1})^{\text{ext}} - (\tilde{f}_{lb}^{n+1})^{\text{int}} - (\tilde{f}_{lb}^{n+1})^{\text{damp}} \right)$$  \hspace{1cm} (5.28)

Introducing the central difference method, the advancement of nodal quantities to $t_{n+1}$ is expressed as:

$$\Delta \tilde{t}_{la}^{n+1} = \Delta t \tilde{v}_{la}^{n+1} + \frac{1}{2} \Delta t^2 \tilde{a}_{la}^{n+1}$$  \hspace{1cm} (5.29)

$$\Delta \tilde{t}_{lb}^{n+1} = \Delta t \tilde{v}_{lb}^{n+1} + \frac{1}{2} \Delta t^2 \tilde{a}_{lb}^{n+1}$$  \hspace{1cm} (5.30)

$$v_{la}^{n+1} = v_{la}^n + \Delta t \tilde{a}_{la}^{n+1}$$  \hspace{1cm} (5.31)

$$v_{lb}^{n+1} = v_{lb}^n + \frac{1}{2} \Delta t \tilde{a}_{lb}^{n+1}$$  \hspace{1cm} (5.32)

Note that the nodal masses $m_{la}^{n+1}$ and $m_{lb}^{n+1}$ are equal to the nodal masses $\tilde{m}_{la}^{n+1}$ and $\tilde{m}_{lb}^{n+1}$, respectively:

$$m_{la}^{n+1} = \tilde{m}_{la}^{n+1}$$  \hspace{1cm} (5.33)

$$m_{lb}^{n+1} = \tilde{m}_{lb}^{n+1}$$  \hspace{1cm} (5.34)

The displacement field $u^h(x)$ can then be updated incrementally by re-interpolating the updated nodal values:
The proposed scheme only requires the mapping of the nodal velocity between different referenced configurations, while the nodal accelerations are obtained by using the equilibrium conditions and the nodal displacements are directly determined by using explicit time integration formulation. The proposed method guarantees the conservation laws of linear momentum and kinetic energy, which follows the classic rules of the physics of a dynamic system.

5.3 A High Order Stabilized Conforming Nodal Integration for Galerkin Meshfree Approximation

Another issue for modeling the crack propagation by meshfree method is domain integration in the Galerkin approximation. The computational cost for domain integration is intensive as the near-tip field enrichment schemes are employed.

Here we start with a boundary value problem (BVP) with fracture:

\[
(u^h(x))^{n+1} = (u^h(x))^n + \sum_{i} \Psi_i^h(x) \Delta d_I^{n+1}
\]  \hspace{1cm} (5.35)

The proposed scheme only requires the mapping of the nodal velocity between different referenced configurations, while the nodal accelerations are obtained by using the equilibrium conditions and the nodal displacements are directly determined by using explicit time integration formulation. The proposed method guarantees the conservation laws of linear momentum and kinetic energy, which follows the classic rules of the physics of a dynamic system.

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Here we start with a boundary value problem (BVP) with fracture:

\[
\nabla \cdot \sigma = -b \text{ in } \Omega, \quad \sigma = C \cdot \nabla u \\
\sigma \cdot n = t \text{ on } \partial \Omega_h, \quad \sigma \cdot n = h \text{ on } \partial \Omega_c \\
u = g \text{ on } \partial \Omega_g
\]

where \(\mathbf{u}\) and \(\sigma\) are the displacement and stress fields, \(C\) is the material moduli tensor, \(\mathbf{t}\) is the surface traction on the Neumann boundary \(\partial \Omega_h\), \(\mathbf{g}\) is the prescribed displacement on the Dirichlet boundary \(\partial \Omega_g\), and \(\mathbf{h}\) is the cohesive traction on the crack surface \(\partial \Omega_c\) as detailed in Figure 5.5.
By applying Galerkin approximation and introducing the extrinsically enriched RK approximation of (5.1) or (5.6), the weak formulation is constructed by multiplying a test function on both sides of the governing equation:

\[
\left( \Psi_f, \nabla \cdot (C : \nabla u^h) \right)_\Omega = - \left( \Psi_f, b \right)_\Omega \quad (5.37)
\]

where \((\cdot, \cdot)\) denotes the \(L_2\) inner product of its two arguments. By performing integration by parts and employing the divergence theorem for the left-hand-side of (5.37), we have:

\[
\left( \Psi_f, \nabla \cdot (C : \nabla u^h) \right)_\Omega = \left( \Psi_f, C : \nabla u^h \cdot n \right)_{\partial \Omega} - \left( \nabla \Psi_f, C : \nabla u^h \right)_\Omega \quad (5.38)
\]

where the relationships between the surface traction terms and deformation are derived as:

\[
\left( \Psi_f, C : \nabla u^h \cdot n \right)_{\partial \Omega} = \left( \Psi_f, t \right)_{\partial \Omega} \quad (5.39)
\]

\[
\left( \Psi_f, C : \nabla u^h \cdot n \right)_{\partial \Omega} = \left( \Psi_f, h \right)_{\partial \Omega} \quad (5.40)
\]

By substituting (5.37), (5.39) and (5.40) into (5.38), the weak formulation has the following expression:

\[
\left( \nabla \Psi_f, C : \nabla u^h \right)_\Omega = \left( \Psi_f, t \right)_{\partial \Omega} + \left( \Psi_f, h \right)_{\partial \Omega} + \left( \Psi_f, b \right)_\Omega 
\]

Furthermore, to restore coercivity of the weak formulation, the essential boundary condition is imposed into (5.41):
\[
(\nabla \Psi_i, C : \nabla u^h)_{\Omega} = (\nabla \Psi_i, t)_{\partial\Omega} + (\nabla \Psi_i, h)_{\partial\Omega} + (\nabla \Psi_i, b)_{\Omega} + \beta (\nabla \Psi_i, u^h - g)_{\partial\Omega} \tag{5.42}
\]

Where $\beta$ is the penalty parameter. Note that the shape function $\Psi_i$ includes both the enriched and un-enriched parts of the approximation as defined in (5.6). The weak formulation is employed to find $u \in U$, for all $\delta u \in V$, where $U$ and $V$ are the proper Sobolev spaces associated with the strong form in (5.36). Rearranging (5.38), the bilinear form satisfies the following conditions:

\[
(\nabla \Psi_i, C : \nabla u^h)_{\Omega} = (\nabla \Psi_i, C : \nabla u^h \cdot n)_{\Omega} - (\nabla \Psi_i, \nabla \cdot (C : \nabla u^h))_{\Omega} \tag{5.43}
\]

The weak form in (5.42) is valid if and only if the domain and boundary integrations satisfy (5.43). Typically, the domain integration of the Galerkin weak formulation is numerically carried out by the Gauss quadrature rule. The Gauss quadrature rule can achieve integration exactness for polynomial functions. Since the RK shape functions are rational and the near-tip enrichment functions are singular in LEFM or highly nonlinear as cohesive zone model or the visibility criteria are adopted, the conventional Gauss quadrature cannot guarantee the exactness of the integration constraint in (5.43).

Chen et al. [105, 106] and Rüter et al. [107] demonstrated that the optimal convergence can be achieved by enforcing variational consistency of Galerkin formulation. It was shown that the solution errors of PDEs due to quadrature inaccuracy can be significantly reduced when the conventional integration methods such as Gauss quadrature or direct nodal integration are corrected via enforcing variational consistency. Consequently the optimal convergence rate can be either partially or fully restored. Following the guidance in the literature [105-107], we will enforce the variational consistency to the domain integration on the left-hand side of (5.43), although the integration exactness is still not fully fulfilled.

Assume the approximated solution of the displacement field is an $n$-th order polynomial:
\[ \mathbf{u}^h = \mathbf{u}^e = \sum_{a=0}^{\alpha} c \mathbf{x}^a \]  

(5. 44)

where \( \mathbf{c} \) is an arbitrary constant vector. Then,

\[ \mathbf{C} : \nabla \mathbf{u}^e = \sum_{a=0}^{\alpha} \mathbf{c} \nabla \mathbf{x}^a = \mathbf{H}(\mathbf{x}) \mathbf{D} \]  

(5. 45)

in which \( \mathbf{C} \) is the elasticity tensor, \( \mathbf{D} \) is the coefficient vector and \( \mathbf{H}(\mathbf{x}) \) is a complete monomial vector expressed (in 2-D) as:

\[ \mathbf{H}(\mathbf{x}) = \{1 \, x \, y \, ... \, x^p y^q\}, \, p + q = n - 1 \]  

(5. 46)

Substituting (5.45) into (5.43) for an arbitrary \( \mathbf{D} \), we have

\[ (\nabla \Psi, \mathbf{H}(\mathbf{x}))_{\Omega} = (\Psi, \mathbf{H}(\mathbf{x}) n)_{\Omega} - (\nabla \Psi, \nabla \cdot \mathbf{H}(\mathbf{x}))_{\Omega} \]  

(5. 47)

The above equation was so-called integration constraints proposed by Chen et al. [105, 106]. The authors of [106] defined the integration constraints as "the integration constraint states that the numerical integration of the domain and boundary integrals for Galerkin approximation of a PDE has to be consistent with the test functions \( \Psi \) in the form of (5.47) for an \( n \)-th order complete numerical method to achieve the \( n \)-th order exactness in the Galerkin approximation". Let the integration domain be divided into multiple conforming nodal domains as

\[ \Omega = \bigcup_{L=1}^{NP} \Omega_L \text{ and } \Omega_i \cap \Omega_j = \emptyset, \text{ as } i \neq j \]  

(5. 48)

where \( \Omega_L \) denotes the conforming nodal domain. An example of the conforming nodal domains is illustrated in Figure 5.6. Consequently, the domain integration of the left-hand side of (5.47) can be rewritten as:

\[ (\nabla \Psi, \mathbf{H}(\mathbf{x}))_{\Omega} = \sum_{L=1}^{NP} (\nabla \Psi, \mathbf{H}(\mathbf{x}))_{\Omega_L} \]  

(5. 49)
To achieve the $n$-th order integration constraints, an integration method is proposed with imposition of the integration constraints on each decomposed subdomain. Let us design the scheme to enforce the integration constraints in each nodal domain $\Omega_L$. Assume that a smoothed gradient $\nabla_L \Psi_L(x)$ in the nodal domain $\Omega_L$ has the following form:

$$\nabla_L \Psi_L(x) = b_L^T H(x) \quad (5.50)$$

where $b_L^T$ is the coefficient vector to be determined with respect to the smoothed gradient $\nabla_L \Psi_L$ in the nodal domain $\Omega_L$.

![Figure 5.6 Geometrical definition of a nodal domain](image)

By imposing the integration constraints to each nodal domain $\Omega_L$ for the smoothed gradient, we have

$$\left( \nabla_L \Psi_L(x), H(x) \right)_{\Omega_L} = \left( \Psi_L(x), H(x) \right)_{\partial \Omega_L} - \left( \Psi_L(x), \nabla \cdot H(x) \right)_{\Omega_L} \quad (5.51)$$

Substituting (5.50) into (5.51), we have

$$\left( b_L^T H(x), H(x) \right)_{\Omega_L} = \left( \Psi_L(x), H(x) \right)_{\partial \Omega_L} - \left( \Psi_L(x), \nabla \cdot H(x) \right)_{\Omega_L} \quad (5.52)$$

Since $b_L^T$ is independent of $x$, it can be obtained by solving the following linear system of equations:

$$b_L^T M_L = Q_L^T \quad (5.53)$$
where

\[ M_L \equiv \left( H^T(x), H(x) \right)_\Omega_c \]  \hspace{1cm} (5.54)

and

\[ Q^L_i \equiv \left( \nabla \Psi_j(x), H(x) \right)_{\partial \Omega_c} - \left( \nabla \Psi_j(x), \nabla H(x) \right)_{\Omega_c} \]  \hspace{1cm} (5.55)

The coefficient \( b^L_i \) can be solved by:

\[ b^L_i = Q^L_i M^{-1}_L \]  \hspace{1cm} (5.56)

Substituting (5.56) into (5.50), the smoothed gradient can then be obtained:

\[ \tilde{\nabla}_L \Psi_j(x) = Q^L_i M^{-1}_L H^T(x) \]  \hspace{1cm} (5.57)

As a result, the domain integration can be carried out as

\[ \left( \nabla \Psi_j, C : \nabla u^h \right)_\Omega = \sum_{j=1}^{NP} \sum_{L=1}^{NP} \left( \tilde{\nabla}_L \Psi_j(x), C : \tilde{\nabla}_L \Psi_j(x) d_j \right)_\Omega_c \]  \hspace{1cm} (5.58)

**Remark 5.1**

It’s straightforward to show that the integration constraints of (5.47) can be satisfied as we introduce the smoothed gradient to the Galerkin approximation. To show the proof, first replace \( \nabla \Psi_j \) by \( \tilde{\nabla}_L \Psi_j(x) \) in the left-hand side of (5.47) and consider only the nodal domain \( \Omega_c \):

\[ \left( \tilde{\nabla}_L \Psi_j(x), H(x) \right)_{\Omega_c} = \left( Q^L_i M^{-1}_L H^T(x), H(x) \right)_{\Omega_c} \]  \hspace{1cm} (5.59)

Since \( Q^L_i \) and \( M^{-1}_L \) are independent of \( x \), we have

\[ \left( \tilde{\nabla}_L \Psi_j(x), H(x) \right)_{\Omega_c} = Q^L_i M^{-1}_L \left( H^T(x), H(x) \right)_{\Omega_c} = Q^L_i M^{-1}_L M_L = Q^L_i \]  \hspace{1cm} (5.60)

Substituting (5.55) into (5.60) and assembling all the sub-domains, we obtain
As the condition of (5.48) holds, the first term of the right-hand-side of (5.61) has the following properties:

$$\sum_{L=1}^{NP} \left( \nabla \Psi_l (x), H(x) \right)_{\partial \Omega_L} = \sum_{L=1}^{NP} \left( \nabla \Psi_l (x), H(x) n \right)_{\partial \Omega_L} - \sum_{L=1}^{NP} \left( \nabla \Psi_l (x), \nabla H(x) \right)_{\Omega_L} \quad (5.61)$$

Consequently,

$$\sum_{L=1}^{NP} \left( \nabla \Psi_l (x), H(x) n \right)_{\partial \Omega_L} = 0, \text{ for all interior nodes } \{ I : \text{ supp } (\nabla \Psi_l) \cap \partial \Omega = \emptyset \} \quad (5.62)$$

Consequently,

$$\sum_{L=1}^{NP} \left( \nabla \Psi_l (x), H(x) n \right)_{\partial \Omega_L} = \left( \nabla \Psi_l (x), H(x) n \right)_{\partial \Omega} \quad (5.63)$$

and

$$\sum_{L=1}^{NP} \left( \nabla \Psi_l (x), \nabla H(x) \right)_{\Omega_L} = \left( \nabla \Psi_l (x), \nabla H(x) \right)_{\Omega} \quad (5.64)$$

Substituting (5.63) and (5.64) into (5.61) and performing integration by parts and the divergence theorem, eventually we prove that the integration constraints of (5.47) are satisfied:

$$\sum_{L=1}^{NP} \left( \nabla \Psi_l (x), H(x) \right)_{\Omega_L} = \left( \nabla \Psi_l, H(x) n \right)_{\partial \Omega} - \left( \nabla \Psi_l, \nabla H(x) \right)_{\Omega} = \left( \nabla \Psi_l, H(x) \right)_{\Omega} \quad (5.65)$$

This concludes the smoothed gradient defined in (5.57) meets integration constrains (5.47) for nodal integration.

**Remark 5.2**

The smoothed gradient contains no derivatives of the shape functions, which can significantly reduce the computational cost for integrating the weak form, since the derivatives of the RK shape functions require complicated calculation due to the rationality. Furthermore, as the
highest order $n$ reduces to 1, meaning that the monomial vector $H(x)$ reduces to a scalar constant, i.e. $H(x) = \{1\}$, the proposed integration method reduces to the standard stabilized conforming nodal integration (SCNI), which was proposed by Chen et al. [105]. Lastly, the corresponding stiffness matrix remains symmetric. Hence, there is no extra cost for solving the linear system of equations.

5.4 Numerical Verification of Benchmark Problems

For the purpose of verifying the proposed model, two benchmark numerical examples are conducted to demonstrate the performance of the proposed enrichment method and four more examples are performed for the proposed domain integration scheme for static linear elastic fracture mechanics and cohesive zone model. In the following examples, the extrinsically enriched RKPM with linear polynomial based shape functions is adopted for all of the numerical simulations.

5.4.1 Stationary and Moving Mode I Crack Problems

An infinite plate with a semi-infinite crack is subjected to a constant tensile stress from above. This problem is given an analytical solution for an imposed crack propagation velocity by Freund [59]. For the purpose of verifying the numerical algorithm, a model with finite dimensions as shown in Figure 5.7 is employed, where the analytical solution of an infinite plate is only valid before the reflected wave from the bottom reaches the crack tip. Hence, the numerical result will be compared for time $t \leq 3t_c = 3h/c_1$, where $c_1 = \sqrt{(\lambda + 2\mu)/\rho}$ is the dilatational wave speed. In this case, plane strain assumption is employed. The crack is
stationary at $t \leq 1.5t_c$ and then propagates with a constant velocity 1,500 m/s. In the numerical model, the tensile stress applied on the top surface is $\sigma_0 = 500$ MPa, the length $L = 10$ m, the initial crack length $a = 5$ m, and the vertical position of the crack is $h = 2$ m. For the material properties, Young’s modulus $E = 210$ GPa, Poisson’s ratio $\nu = 0.3$ and the density $\rho = 8000$ kg/m$^3$.

The numerical results obtained by using the presented methods are plotted in Figure 5.8. A 3-D model with 121x60x2 nodes is used. The numerical results are compared with the analytical solution and the one from Menouillard et al. [55] by using the 2-D XFEM of 121x60 nodes with explicit time integration scheme. Since a 2-D plane strain assumption is made in this problem, all the degrees of freedom at the thickness direction are fixed to represent the 2-D plane strain condition. As can be seen from Figure 5.8, the numerical results are quite smooth for the stationary crack but show oscillations after imposing the constant crack propagation velocity. The solution of the XFEM even shows larger oscillations. These oscillations were also observed by the authors in the literature [54-56]. Although the numerical simulation shows oscillations, the overall numerical results still agree well with the analytical solution.

![Figure 5.7 Semi-infinite crack in an infinite plate subjected to a tensile stress wave](image)
5.4.2 An Edge-cracked Plate under Impulsive Loading

As shown in Figure 5.9, a plate with two symmetric edge notches is impacted by a projectile at speed $v_0$. This example is based on the Kalthoff's experiments [60]. In this model, the two cracks are located in a symmetrical position about the center line of the plate with the same crack length. The projectile is launched to impact on the left boundary between the two cracks. This is a mixed-mode problem for testing the capability of the proposed method, which shows a more complicated crack propagation path. In this case, $v_0=20$ m/s is used as a typical velocity for brittle fracture. The critical stress intensity factor $K_{1c}=68$ MPa is used for crack propagation criterion. For the material properties, Young’s modulus $E=190$ GPa, Poisson's ratio $\nu=0.3$ and the density $\rho=8000$ kg/m$^3$ are used. The dilatational wave speed $c_d=5654.3$ m/s; the shear wave speed $c_s=3022.4$ m/s; and the Rayleigh wave speed $c_r=2799.2$ m/s.

In this case, a half model symmetrical about the center line is adopted to conduct the numerical simulation. Plane strain assumption is also used in this example. Maximum hoop stress criterion [41] is chosen to determine the crack propagation angle. The crack propagation velocity is determined by the following equation which is suggested by Freund [61]:

$$v_c = \frac{K_{1c}}{\sigma_0 \sqrt{h}}$$
\[ v_{cra} = \begin{cases} 
0 & \text{if } K_{\theta \theta} < K_{1c} \\
c_i \left(1 - \frac{K_{1c}}{K_{\theta \theta}}\right) & \text{otherwise}
\end{cases} \quad (5.66) \]

where \( v_{cra} \) is the crack propagation speed, \( K_{1c} \) is the critical value of the mode I stress intensity factor, and \( K_{\theta \theta} \) is the equivalent dynamic stress intensity factor. A 79x79x2-node model is constructed to simulate this problem. Figure 5.10 shows the crack's final path from the numerical result. From the experiment by Kalthoff, the overall crack angle is about 70°, while the numerical one shows an average angle of about 67.6°, which agrees well with the experimental result. The result also demonstrates the capability of the proposed method to deal with kinked crack propagation.

Figure 5.9 The schematic description of the edge-cracked plate under impulsive loading

Figure 5.10 The final crack path for the edge-cracked plate
5.4.3 Convergence Study of Motz's Problem

Motz's problem was first discussed by Motz [108] in 1947, which was later employed as a benchmark for singularity problems to compare the effectiveness of numerical methods. Motz's problem solves the Laplace's equation on a rectangular domain \( \Omega \):

\[
\Delta u = 0 \text{ in } \Omega, \quad \Omega \in [-1,1] \times [0,1] \tag{5.67}
\]

where \( \Delta = \nabla^2 \) is the Laplace operator and \( u \) is a function in terms of the 2-D coordinates \( x, y \) in which \( x \in \Omega \). The singularity of the solution \( u \) is introduced by imposing mixed Neumann–Dirichlet boundary conditions as illustrated in Figure 5.11.

![Figure 5.11 The boundary conditions of Motz's Problem](image)

The singularity exists at the origin \((0,0)\) due to the intersection of the Neumann–Dirichlet boundary conditions. The analytical solution can be found in the literature [109], which is expressed as an expansion form in terms of the polar coordinates \( r \) and \( \theta \):

\[
 u(r, \theta) = \sum_{i=0}^{\infty} a_i r^{i+0.5} \cos(i + 0.5)\theta \tag{5.68}
\]

Taking derivatives for the solution \( u \), one can find that the singularity is included in the first
term as \( r \) approaches 0. The problem will be solved by using Galerkin approximation. We introduce the first term of the expansion (5.68) as an enrichment basis in addition to the RK approximation with linear order of basis functions:

\[
    u = \sum_{i=1}^{NP} \Psi_i(x)\xi_i + a_0\sqrt{r}\cos\frac{\theta}{2}
\]  

(5.69)

Here, the numerical simulations for Motz's problem are conducted to demonstrate the performance of the proposed high order SCNI for domain integration of Galerkin approximation for problem with singularity. The convergence curves of the L2 and semi-H1 error norms, normalized by the norms of the solution, are plotted in Figure 5.12 and Figure 5.13, respectively. Comparisons are made among different integration schemes. They are the first order and the second order SCNI and the standard 5-point Gauss quadrature rule. For the first and second order SCNI, 2-point and 3-point Gauss Lobatto quadrature rules are employed to integrate the vector \( \mathbf{Q} \) and the moment matrix \( \mathbf{M} \) shown in (5.55) and (5.54), respectively. The 2-point and 3-point Gauss Lobatto quadrature rules can achieve first order and second order integration exactness respectively, which include the boundary points of the integration cell. The convergence rates for the corresponding integration methods are also marked in the plots. As can be seen from the comparison, the first order SCNI does not achieve the regular convergence rate for L2 norm and Semi-H1 norms, since it only has the first order accuracy for the domain integration, which is not sufficient for the singular base function. As the second order SCNI is used, the regular convergence rate is restored. With the linear basis RK approximation, the convergence rates for L2 and semi-H1 norms should be 1.5 and 0.5, respectively. Furthermore, the accuracy by using the second order SCNI is close to the one using standard 5-point Gauss quadrature rule, but the computational cost for the proposed high order SCNI is lower, since only the minimum required 3 integration points are used in the second order SCNI.
5.4.4 A Stationary Edge-crack Problem

Consider an edge-cracked plate whose dimensions and boundary condition are illustrated in Figure 5.14. For the material properties, the Young’s modulus $E=100,000$ psi, Poisson's ratio $\nu=0.3$ and the plane strain assumption are adopted in this problem. Due to symmetry, we only model half of the plate. The exact solution of this problem with a stationary crack is given by [110], as
\[ K_1 = C \sigma \sqrt{a \pi} \]  

(5. 70)

where \( a = 3.5 \) in. is the crack length and \( C \) is a finite-geometry correction factor:

\[
C = 1.12 - 0.231 \left( \frac{a}{W} \right) + 10.55 \left( \frac{a}{W} \right)^2 - 21.72 \left( \frac{a}{W} \right)^3 + 30.39 \left( \frac{a}{W} \right)^4
\]

(5. 71)

in which \( W = 7.0 \) in. is the width of the plate.

Two different uniform discretizations with 21x21 and 41x41 nodes are used to compare the efficiency of the proposed integration scheme with the conventional Gauss quadrature for the extrinsically enriched RKPM. For the numerical simulations, linear bases with a normalized support size 1.5 is used for all the discretizations. The results are shown in Figure 5.15. The mode I stress intensity factors with different order integration methods are compared. Note that the y-axis in Fig. 5.15 denotes the number of the integration points in one dimension, e.g., 2 points mean 2x2 points used in each nodal domain. For the proposed integration method, the Gauss-Lobatto quadrature is used to integrate the vector \( \mathbf{Q} \) and the moment matrix \( \mathbf{M} \), which includes the boundary quadrature points. The numbers of integration points used for the first order to the third order Gauss-Lobatto quadrature are 2x2 to 4x4 points, respectively. The numbers of the points are the minimum requirements for the corresponding integration orders. The stress intensity factors are computed using domain forms of the interaction.
integrals [111-112]. In Figure 5.15, the proposed integration scheme shows better accuracy of the mode I intensity factor than the conventional Gauss quadrature rule under the same number of quadrature points.

![Graph showing comparison of K1 under different integration schemes](image)

**Figure 5.15 Comparison of K1 under different integration schemes**

Another comparison is made between the extended finite element method (XFEM) and the extrinsically enriched RKPM as shown in Table 5.1. For XFEM, 8x8 Gauss quadrature points are used for the domain integration, while for RKPM, the third order SCNI with 4x4 Gauss-Lobatto quadrature points is adopted. Four different discretizations are compared for the nodal spacing from h=1 in. to 1/8 in. To ensure a fair comparison, the domains of the interaction integral for evaluating the stress intensity factors are the same for the XFEM and RKPM simulations. The results of RKPM shows better accuracy than the ones of XFEM in the evaluation of the intensity factor as the discretization is refined. This is most likely due to the fact that the RK shape functions are smoother than the finite element shape functions.

**Table 5.1 Comparison of error in K1 (%) using RKPM with higher order SCNI and XFEM**

<table>
<thead>
<tr>
<th>h (in)</th>
<th>1</th>
<th>1/2</th>
<th>1/4</th>
<th>1/8</th>
</tr>
</thead>
<tbody>
<tr>
<td>RKPM</td>
<td>3.413</td>
<td>1.199</td>
<td>0.416</td>
<td>-0.012</td>
</tr>
<tr>
<td>XFEM</td>
<td>-2.513</td>
<td>-1.269</td>
<td>-0.574</td>
<td>-0.290</td>
</tr>
</tbody>
</table>
5.4.5 A Three-point Bending Specimen with Cohesive Zone Modeling

Consider a three-point bending beam shown in Figure 5.16. This case has been studied by Carpinteri and Colombo [113] for the consideration of a cohesive crack growth in such a specimen by using the finite element analysis and the node release technique. The dimensions of the beam are illustrated in Figure 5.16, where the thickness is 0.15 m, which is the same as the depth of the beam. For the material properties, Young’s modulus $E=36.5$ GPa, Poisson's ratio $\nu=0.1$, and the cohesive strength $f_u=3.14$ MPa are used. Linear cohesive law is chosen with the fracture energy $G_F = 50$ N/m and the plane stress assumption is adopted in this problem. A uniform discretization of 61x16 nodes is used to model the problem. Initially, there is no pre-crack in the specimen. The crack in the bottom middle of the beam is initiated as the maximum tensile stress reaches the cohesive strength $f_u$. Due to the symmetry of the loading condition and specimen geometry, we know this case is a pure mode I problem. We compared the numerical results between RKPM and FEM. The load–deflection curves are shown in Figure 5.17, where the solution of RKPM agrees well with the solution of finite element method. Through the comparison, we confirm the reliability of the solution from extrinsically enriched RKPM for cohesive zone modeling.

![Figure 5.16 A three-point bending beam](image-url)
5.4.6 A Single Edge Notched Beam

This case is chosen to test the proposed extrinsically enriched RKPM for mixed-mode fracture. The dimensions of this problem are shown in Figure 5.18. For the material properties, Young’s modulus $E=38$ GPa, Poisson’s ratio $\nu=0.18$, and the cohesive strength $f_u=3.0$ MPa are used. Linear cohesive law is chosen with the fracture energy $G_F = 69$ N/m and the plane stress assumption is adopted in this problem. This problem is designed to study load–deflection behavior and crack paths of concrete specimens subjected to non-proportional loading [114-115]. A uniform discretization of 163x37 nodes is used for numerical simulation. The numerical result of RKPM is compared with the one by Areias and Belytschko [116], who used the 3-D crack modeling under the framework of the XFEM to solve this problem. As shown in Figure 5.19, the load-COD (crack opening displacement) curve of RKPM agrees well with the result of the XFEM, which demonstrates that the solution of the extrinsically enriched RKPM is reliable for modeling mixed mode crack propagation.
Figure 5.18 A single edge notched beam

Figure 5.19 Load-COD curves of the mixed mode fracture problem
Chapter 6

The Stochastic Multi-scale Modeling

In this chapter, the conventional multi-scale methods are reviewed first. The so-called stochastic representative volume element (SRVE) [89-94, 117-119] is then discussed, and finally some numerical results based on a set of CT scans of concrete material are conducted to demonstrate the existence of the SRVE. Two classical approaches for multi-scale homogenization will be discussed: the asymptotic expansion based multi-scale methods [71, 83, 120-123] and the energy equivalence approaches with various prescribed boundary conditions [82, 89-93, 124]. As the homogenized material properties of heterogeneous microstructures are derived, the randomness of the micro-structural geometry and material properties is introduced based on stochastic theories.

6.1 The Characteristics of the Stochastic Representative Volume Element

The definition of SRVE was given by Hill [89], who described the existence of SRVE as "(a) entirely typical of the whole mixture on average and (b) contains a sufficient number of inclusions for the overall moduli to be effectively independent of the surface values of traction and displacement, so long as these values are macroscopically uniform". The statement of (a) is about the material's statistical nature, while (b) describes that the effective
material moduli should be independent of the prescribed boundary conditions in the macro-scale. Generally speaking, the following conditions are required to be satisfied for the SRVE to exist:

1. The micro-structure is periodic in a random sense.
2. The given micro-structure is sufficiently large so that the RVE is statistically representative for the entire micro-structure. When the volume of the microscopic base cell is smaller than the RVE, a representative property cannot be defined and the continuum description of the material breaks down.
3. The spatial correlation lengths of the mechanical fields in the micro-structure are small enough with respect to the dimension of the macro-structure.

To describe the characteristics of SRVE, three conditions are considered, the Hill condition, ergodicity and the principle of the minimum potential energy. The first two are assumptions for SRVE with certain stochastic properties and sufficiently rich microstructural information, and the last one is the nature of the continuum mechanics. The details will be addressed in the following sections.

Hill [89] defined the following condition for heterogeneous elastic materials:

\[ \overline{\boldsymbol{\sigma}} : \varepsilon = \overline{\varepsilon} : \overline{\varepsilon} \]  \hspace{1cm} (6.1)

where \( \sigma = \sigma(x) \) and \( \varepsilon = \varepsilon(x) \) are stresses and strains in terms of spatial coordinates, and the overbar "—" denotes the operator of the spatial average defined as follows:

\[ \overline{f} = \frac{1}{V} \int_{\Omega} f(x) d\Omega \]  \hspace{1cm} (6.2)

in which \( \Omega \) is the occupied domain, \( V \) is the volume of the occupied domain.

The condition in (6.1) was then named after Hill as "Hill condition". It is well known in the classical mechanics that two types of boundary conditions satisfy the Hill condition (6.1). They are the pure Dirichlet boundary and pure Neumann boundary conditions with zero body
forces. The first one corresponds to prescribing displacements $u^D_{\Omega}$ on the entire boundary $\partial \Omega$ of the microscopic cell with the occupied domain $\Omega$ in the following form:

$$u^D_{\Omega} = \varepsilon_0 \cdot x \text{ on } \partial \Omega$$  \hspace{1cm} (6.3)

where the superscript "$D$" denotes that the quantities are under the Dirichlet boundary condition, $\varepsilon_0$ is the homogenized strain tensor and $x$ is the spatial coordinates. Note that the homogenized strain is equal to the spatially averaged strain over the domain $\Omega$ if there is no internal cracks in the body:

$$\bar{\varepsilon}^D_{\Omega} = \frac{1}{V} \int_\Omega \varepsilon^D_{\Omega} \, d\Omega = \frac{1}{2V} \int_{\partial\Omega} (u^D_{\Omega} \otimes n + n \otimes u^D_{\Omega}) \, d\Gamma = \varepsilon_0$$  \hspace{1cm} (6.4)

Now, consider the internal energy density under the prescribed boundary condition:

$$U = \frac{1}{2} \sigma^D_{\Omega} : \varepsilon^D_{\Omega} = \frac{1}{2V} \int_{\partial\Omega} \sigma^D_{\Omega} : \varepsilon^D_{\Omega} \, d\Omega$$  \hspace{1cm} (6.5)

With zero body force, $U$ can be transformed from domain integral into boundary integral through divergence theorem and integration by parts:

$$U = \frac{1}{2V} \int_{\partial\Omega} \sigma^D_{\Omega} : \frac{1}{2} (n \otimes (\varepsilon_0 \cdot x) + (\varepsilon_0 \cdot x) \otimes n) \, d\Gamma$$  \hspace{1cm} (6.6)

Substituting (6.3) into (6.6), we have

$$U = \frac{1}{2V} \int_{\partial\Omega} \sigma^D_{\Omega} : \frac{1}{2} \left(n \otimes \varepsilon_0 + \varepsilon_0 \otimes n\right) = \frac{1}{2} \sigma^D_{\Omega} : \bar{\varepsilon}^D_{\Omega}$$  \hspace{1cm} (6.7)

Simply put,

$$U = \frac{1}{2} \sigma^D_{\Omega} : \varepsilon^D_{\Omega} = \frac{1}{2} \sigma^D_{\Omega} : \bar{\varepsilon}^D_{\Omega}$$  \hspace{1cm} (6.8)

To estimate random material properties via observations on specific samples, one needs to consider the concept of ergodicity. The classical ergodic concept stemmed from the dynamic systems of statistical physics. If the dynamic system is ergodic, it has the same
behavior averaged over time as averaged over the space of all the system's states. In the field of SRVE, ergodicity describes the condition of a random process for which the spatial average is the same as the ensemble average of the sequence of the events:

\[
\bar{f} = \lim_{V \to \infty} \frac{1}{V} \int_V f(x, \theta) \, d\Omega = \int_{\Theta} f(x, \theta) \rho(\theta) \, d\theta = \langle f \rangle
\]  (6. 9)

where \( \theta \) is the random variable in the probability space, \( \langle \bullet \rangle \) denotes the operator of the ensemble average, \( \Theta \) is the concerned domain in the probability space and \( \rho(\theta) \) is the probability density function.

The above equation implies that the occupied domain of the microscopic cell should be very large (mathematically infinite) compared with the size of micro-scale elements, such that the microscopic cell can be considered as the SRVE, which is statistically representative for the entire micro-structure.

To specifically describe the characteristics of ergodicity, one can find an example of the function \( f \) which possesses the ergodic property:

\[
f(x, \theta) = c_1 + c_2 \sin \left( \frac{2\pi}{l_0} x \right) \sin \left( \frac{2\pi}{l_0^\theta} \theta \right)
\]  (6. 10)

where \( c_1 \) and \( c_2 \) are constants and \( l_0 \) and \( l_0^\theta \) are the wavelengths of the sinusoidal function as illustrated in Figure 6.1. In the probabilistic domain, we assume the probability density function of \( \theta \) is uniform over the length \( 2n l_0^\theta \):

\[
\rho(\theta) = \frac{1}{2n l_0^\theta}
\]  (6. 11)

The spatial average of \( f(x, \theta) \) over the length \( 2n l_0^s \) can then be written as:

\[
\lim_{m \to \infty} \frac{1}{2n l_0^s} \int_{-m l_0^s}^{m l_0^s} f(x, \theta) \, dx = \lim_{m \to \infty} \frac{1}{2n l_0^s} \int_{-m l_0^s}^{m l_0^s} \left[ c_1 + c_2 \sin \left( \frac{2\pi}{l_0} x \right) \sin \left( \frac{2\pi}{l_0^\theta} \theta \right) \right] \, dx
\]  (6. 12)
Note that the second term in the right hand side of (6.12) will vanish as \( m \to \infty \), since the integral of a sinusoidal function is finite, but the spatial domain is infinite:

\[
\lim_{m \to \infty} \frac{1}{2ml_0} \int_{-ml_0}^{ml_0} \left[ c_2 \sin \left( \frac{2\pi}{l_0^2} x \right) \sin \left( \frac{2\pi}{l_0^2} \theta \right) \right] dx = 0 \quad (6.13)
\]

Therefore, as the concerned domain is sufficiently large, the spatial average of \( f(x, \theta) \) will be a constant \( c_1 \):

\[
\bar{f} = \lim_{m \to \infty} \frac{1}{2ml_0} \int_{-ml_0}^{ml_0} f(x, \theta) dx = c_1 \quad (6.14)
\]

![Figure 6.1 A 2-D sinusoidal of function with infinite domain](image)

On the other hand, the ensemble average of \( f(x, \theta) \) can be written in the following form:

\[
\lim_{n \to \infty} \int_{nl_0^2}^{nl_0^2} f(x, \theta) \rho(\theta) d\theta = \lim_{n \to \infty} \int_{nl_0^2}^{nl_0^2} \left[ c_1 + c_2 \sin \left( \frac{2\pi}{l_0^2} x \right) \sin \left( \frac{2\pi}{l_0^2} \theta \right) \right] \frac{1}{2nl_0^2} d\theta \quad (6.15)
\]

Following the similar derivation, one can find that the ensemble average of the sinusoidal function approaches to 0 as \( n \to \infty \), and the ensemble average can be obtained:
Comparing (6.14) and (6.16), we prove that \( f(x, \theta) \) possesses the ergodic property:

\[
\bar{f} = \langle f \rangle = c_i
\]  

(6.17)

In the multi-scale homogenization, if the fluctuations of the mechanical fields are finite and the concerned spatial and probabilistic domains are sufficiently large, these fields are ergodic. This is because the average of the fluctuations vanish over infinite domains. If the microstructure possesses the ergodic property as shown in (6.9), we can then prove that the stress and strain fields are statistically uncorrelated:

\[
U = \frac{1}{2} \sigma^D \cdot \varepsilon^D = \frac{1}{2} \mathbf{\bar{\sigma}}^D \cdot \mathbf{\bar{\varepsilon}}^D
\]

(6.18)

Alternatively, one can apply the pure Neumann boundary condition on the entire boundary of the microscopic cell:

\[
\mathbf{t}_\Omega^N = \sigma_0 \cdot \mathbf{n} \text{ on } \partial \Omega
\]

(6.19)

where the superscript "N" denotes that the quantities are under the Neumann boundary condition and \( \sigma_0 \) is a constant homogenized stress tensor. Under this type of boundary condition, a similar result can be obtained as the one under the pure Dirichlet boundary condition that the homogenized stress tensor is equal to the spatially averaged stress tensor over the domain \( \Omega \):

\[
\mathbf{\bar{\sigma}}_\Omega^N = \frac{1}{V} \int_V \mathbf{\sigma}_\Omega^N \, d\Omega = \frac{1}{V} \int_{\partial \Omega} \sigma_0 \cdot \mathbf{n} \otimes \mathbf{x} \, d\Gamma = \sigma_0
\]

(6.20)

With zero body force, the internal energy density becomes:

\[
U = \frac{1}{2} \sigma^N \cdot \varepsilon^N = \frac{1}{2V} \int_V \mathbf{\sigma}_\Omega^N \cdot \mathbf{\varepsilon}_\Omega^N \, d\Omega = \frac{1}{2V} \int_{\partial \Omega} \mathbf{t}_\Omega^N \otimes \mathbf{u}_\Omega^N \, d\Gamma
\]

(6.21)
Substituting (6.19) into (6.21), we have:

\[
U = \frac{1}{2V} \int_{\Omega} \sigma_0 : \left( n \otimes u^N_\Omega + u^N_\Omega \otimes n \right) \, d\Gamma
\]

\[
= \frac{1}{2} \sigma_0 : \int_{\Omega} \varepsilon^N_\Omega \, d\Omega = \frac{1}{2} \sigma^N_\Omega : \varepsilon^N_\Omega
\] (6.22)

then comparing (6.21) and (6.22), it is clear that the Hill condition is also satisfied:

\[
U = \frac{1}{2} \sigma^N_\Omega : \varepsilon^N_\Omega = \frac{1}{2} \sigma^N_\Omega : \varepsilon^N_\Omega
\] (6.23)

With the ergodicity, we further obtain:

\[
U = \frac{1}{2} \sigma^N_\Omega : \varepsilon^N_\Omega = \frac{1}{2} \sigma^N_\Omega : \varepsilon^N_\Omega
\]

\[
= \frac{1}{2} \left( \sigma^N_\Omega : \varepsilon^N_\Omega \right) = \frac{1}{2} \left( \sigma^N_\Omega : \varepsilon^N_\Omega \right)
\] (6.24)

As the Hill condition is fulfilled and the microstructure possesses the ergodic property, one can further derive the hierarchies of mesoscale bounds for linear elastic microstructures.

Under the pure boundary conditions (6.3) and (6.19), the internal energy density for a linear problem can be obtained through the calculation of average strains and stresses. The relationships between the average strains and average stresses resulting from the Dirichlet boundary condition can be defined:

\[
\bar{\sigma}^D_\Omega = \tilde{\mathbf{C}}^D_\Omega : \bar{\varepsilon}^D_\Omega
\] (6.25)

where \( \tilde{\mathbf{C}}^D_\Omega \) is the effective stiffness tensor under the Dirichlet boundary condition.

By substituting (6.25) into (6.7), the internal energy density can be rewritten as

\[
U = \frac{1}{2} \bar{\varepsilon}^D_\Omega : \tilde{\mathbf{C}}^D_\Omega : \bar{\varepsilon}^D_\Omega
\] (6.26)

Next, consider a 2-D square domain partitioned into 4 equal-size sub-squares as shown in Figure 6.2. Each sub-domain is defined as \( \Omega_{i}^{\text{sub}} \) with volume \( V_{i}^{\text{sub}} = \frac{1}{4} V \), and \( \bigcup_{i=1}^{4} \Omega_{i}^{\text{sub}} = \Omega \).

The consistent Dirichlet boundary condition is imposed to the boundary of each sub-domain:
The solution fields of the sub-domains are denoted as $\mathbf{u}_{\Omega_{i}^{sub}}^D$, $\sigma_{\Omega_{i}^{sub}}^D$, and $\varepsilon_{\Omega_{i}^{sub}}^D$, which are kinematically admissible. Note that the averaged strains of the sub-domains are the same as the overall averaged strains of the entire domain when the consistent Dirichlet boundary condition is imposed:

$$\bar{\varepsilon}_{\Omega_{i}^{sub}}^D = \varepsilon_0 = \bar{\varepsilon}_{\Omega}^D$$  \hspace{1cm} (6. 28)

The fields of the entire domain follow the previous definitions, i.e. $\mathbf{u}_{\Omega}^D$, $\sigma_{\Omega}^D$, and $\varepsilon_{\Omega}^D$.

To derive the hierarchies of the material moduli, we first introduce the principle of minimum total potential energy. Define $\mathbf{\hat{u}}$ as a perturbation from the equilibrated displacement fields $\mathbf{u}$, and consider a positive functional $F(\mathbf{u}, \mathbf{\hat{u}})$ as follows:

$$F(\mathbf{u}, \mathbf{\hat{u}}) = \frac{1}{2} \int_V (\varepsilon - \hat{\varepsilon}) : \mathbf{C} : (\varepsilon - \hat{\varepsilon}) d\Omega \geq 0$$  \hspace{1cm} (6. 29)

Note $\mathbf{C}$ is a positive definite fourth order tensor, $\varepsilon = \varepsilon(\mathbf{u})$, and $\hat{\varepsilon} = \hat{\varepsilon}(\mathbf{\hat{u}})$. The fields $\hat{\varepsilon}$, $\mathbf{\hat{u}}$, $\varepsilon$ and $\mathbf{u}$ are assumed to be kinematically admissible to the periodic boundary conditions on the sub-divided RVEs and $\sigma (=\mathbf{C}:\varepsilon)$ satisfies the equilibrium conditions. Expanding the left hand side of the inequality, we have
Applying integration by parts and the divergence theorem to the above inequality, the principle of minimum total potential energy with vanishing body force can be obtained:

\[
\frac{1}{2} \int_V \sigma : \varepsilon d\Omega - \int_{\partial V} \mathbf{u} \cdot \mathbf{t} \, d\Gamma \leq \frac{1}{2} \int_V \hat{\sigma} : \hat{\varepsilon} d\Omega - \int_{\partial V} \hat{\mathbf{u}} \cdot \mathbf{t} \, d\Gamma
\]  
(6.31)

The principle states that a body should deform to a configuration that minimizes the total potential energy. The fields \( \hat{\mathbf{e}} \) and \( \hat{\mathbf{u}} \) can be treated as arbitrary perturbations from the fields \( \varepsilon \) and \( \mathbf{u} \) in equilibrium as long as they are kinematically admissible, but \( \hat{\sigma} \) is not necessary to be in equilibrium.

The sub-domain fields \( \mathbf{u}^D_{\Omega_{ia}} \), \( \sigma^D_{\Omega_{ia}} \), and \( \varepsilon^D_{\Omega_{ia}} \) are also kinematically admissible, since the consistent pure boundary conditions are imposed as given in (6.27). Following the principle of minimum potential energy by replacing the perturbation terms in (6.31), we have:

\[
\frac{1}{V} \left( \frac{1}{2} \int_V \varepsilon^D_{\Omega} : \varepsilon^D_{\Omega} \, d\Omega - \int_{\partial \Omega} \mathbf{t}^D_{\Omega} \cdot \mathbf{u}^D_{\Omega} \, d\Gamma \right) \leq \frac{1}{2} \int_V \varepsilon^D_{\Omega} : \varepsilon^D_{\Omega} \, d\Omega - \int_{\partial \Omega} \mathbf{t}^D_{\Omega} \cdot \mathbf{u}^D_{\Omega} \, d\Gamma
\]  
(6.32)

Note the displacement field \( \mathbf{u}^D_{\Omega_{ia}} \) and the surface traction \( \mathbf{t}^D_{\Omega} \) are continuous across the boundary of any two neighboring sub-domains, and \( \mathbf{u}^D_{\Omega} = \mathbf{u}^D_{\Omega_{ia}} \) on the overall boundary of the entire domain, we have:

\[
\int_{\partial \Omega} \mathbf{t}^D_{\Omega} \cdot \mathbf{u}^D_{\Omega} \, d\Gamma = \sum_{i=1}^{4} \int_{\partial \Omega_{ia}} \mathbf{t}^D_{\Omega} \cdot \mathbf{u}^D_{\Omega_{ia}} \, d\Gamma
\]  
(6.33)

Substituting (6.33) into (6.32), the inequality becomes:

\[
\frac{1}{2V} \int_V \varepsilon^D_{\Omega} : \varepsilon^D_{\Omega} \, d\Omega \leq \frac{1}{2V} \sum_{i=1}^{4} \int_{\partial \Omega_{ia}} \varepsilon^D_{\Omega_{ia}} : \varepsilon^D_{\Omega_{ia}} \, d\Omega
\]  
(6.34)
Applying the (6.26) to the sub-domain fields, (6.34) can then be expressed by the linear operation of the average quantities:

$$\frac{1}{2} \mathbf{\bar{e}}^D \mathbf{C}^D : \mathbf{\bar{e}}^D \leq \frac{1}{2} \sum_{i=1}^{4} \frac{1}{4} \mathbf{\bar{e}}^D_{\Omega_{i \alpha}} : \mathbf{C}^D_{\Omega_{i \alpha}} : \mathbf{\bar{e}}^D = \frac{1}{2} \mathbf{\bar{e}}^D : \frac{1}{4} \left( \sum_{i=1}^{4} \mathbf{C}^D_{\Omega_{i \alpha}} \right) : \mathbf{\bar{e}}^D$$

With the assumptions of statistical homogeneity and ergodicity of the material, the average over the four sub-domains can be expressed as:

$$\left\langle \frac{1}{2} \mathbf{\bar{e}}^D : \mathbf{C}^D : \mathbf{\bar{e}}^D \right\rangle \leq \left\langle \frac{1}{2} \mathbf{\bar{e}}^D : \frac{1}{4} \left( \sum_{i=1}^{4} \mathbf{C}^D_{\Omega_{i \alpha}} \right) : \mathbf{\bar{e}}^D \right\rangle$$

(6.36)

Since \( \mathbf{\bar{e}}^D_{\Omega_i} = \mathbf{\bar{e}}^D_{\Omega_{i \alpha}} = \mathbf{\bar{e}}_0 \) are deterministic, (6.36) can be rewritten as:

$$\frac{1}{2} \mathbf{\bar{e}}^D : \left( \mathbf{\bar{C}}^D_{\Omega} \right) : \mathbf{\bar{e}}^D \leq \frac{1}{2} \mathbf{\bar{e}}^D : \frac{1}{4} \left( \sum_{i=1}^{4} \mathbf{\bar{C}}^D_{\Omega_{i \alpha}} \right) : \mathbf{\bar{e}}^D = \frac{1}{2} \mathbf{\bar{e}}^D : \left( \mathbf{\bar{C}}^D_{\Omega/4} \right) : \mathbf{\bar{e}}^D$$

(6.37)

Note that the inequality is defined by the energy which is a scalar. Although \( \mathbf{\bar{e}}^D_{\Omega} \) can be arbitrary, this does not mean that all the components of the stiffness tensor follow the same inequality. However, for some simple cases, such as the isotropic material, the inequality can be used to determine the bounds of the material moduli. The inequality can be expressed as the following form:

$$\frac{1}{2} \left\{ \mathbf{\bar{e}}^D \right\}^T \left[ \left\langle \mathbf{\bar{C}}^D_{\Omega} \right\rangle \right] \left\{ \mathbf{\bar{e}}^D \right\} \leq \frac{1}{2} \left\{ \mathbf{\bar{e}}^D \right\} \left[ \left\langle \mathbf{\bar{C}}^D_{\Omega/4} \right\rangle \right] \left\{ \mathbf{\bar{e}}^D \right\}$$

(6.38)

where \{\bullet\} and [\bullet] denote the quantities as a vector and a matrix, respectively.

Equation (6.38) can be expressed as:

$$\frac{1}{2} \left\{ \mathbf{\bar{e}}^D \right\}^T \left[ \left\langle \mathbf{\bar{C}}^D_{\Omega/4} \right\rangle - \left\langle \mathbf{\bar{C}}^D_{\Omega} \right\rangle \right] \left\{ \mathbf{\bar{e}}^D \right\} \geq 0$$

(6.39)

Since \( \left\{ \mathbf{\bar{e}}^D \right\} \neq \mathbf{0} \), equation (6.40) implies that \( \left[ \left\langle \mathbf{\bar{C}}^D_{\Omega/4} \right\rangle - \left\langle \mathbf{\bar{C}}^D_{\Omega} \right\rangle \right] \) is positive semi-definite.
indicating that all eigenvalues of the matrix form of $\left[\tilde{\mathbf{C}}_{\Omega}^{D}\right]$ are nonnegative.

For an isotropic material:

$$
\left[\left\langle \mathbf{C}_{\Omega}^{D} \right\rangle \right] = \left[ \left[ \left\langle \mathbf{A}^{D} \right\rangle \right] \quad [0] \right],
$$

$$
\left[ \left\langle \mathbf{A}^{D} \right\rangle \right] = \frac{\tilde{E}^{D}_{\Omega}}{(1+v^{D}_{\Omega})(1-2v^{D}_{\Omega})} \begin{bmatrix} 1-v^{D}_{\Omega} & v^{D}_{\Omega} & v^{D}_{\Omega} \\ v^{D}_{\Omega} & 1-v^{D}_{\Omega} & v^{D}_{\Omega} \\ v^{D}_{\Omega} & v^{D}_{\Omega} & 1-v^{D}_{\Omega} \end{bmatrix},
$$

(6. 40)

$$
\left[ \left\langle \mathbf{B}_{\Omega}^{D} \right\rangle \right] = \frac{2\tilde{E}^{D}_{\Omega}}{(1+v^{D}_{\Omega})} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}
$$

For the smaller microscopic cells:

$$
\left[\left\langle \mathbf{C}_{\Omega/4}^{D} \right\rangle \right] = \left[ \left[ \left\langle \mathbf{A}^{D}_{\Omega/4} \right\rangle \right] \quad [0] \right],
$$

$$
\left[ \left\langle \mathbf{A}^{D}_{\Omega/4} \right\rangle \right] = \frac{\tilde{E}^{D}_{\Omega/4}}{(1+v^{D}_{\Omega/4})(1-2v^{D}_{\Omega/4})} \begin{bmatrix} 1-v^{D}_{\Omega/4} & v^{D}_{\Omega/4} & v^{D}_{\Omega/4} \\ v^{D}_{\Omega/4} & 1-v^{D}_{\Omega/4} & v^{D}_{\Omega/4} \\ v^{D}_{\Omega/4} & v^{D}_{\Omega/4} & 1-v^{D}_{\Omega/4} \end{bmatrix},
$$

(6. 41)

$$
\left[ \left\langle \mathbf{B}_{\Omega/4}^{D} \right\rangle \right] = \frac{2\tilde{E}^{D}_{\Omega/4}}{(1+v^{D}_{\Omega/4})} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}
$$

and

$$
\left\{ \mathbf{\bar{\varepsilon}}^{D}_{\Omega} \right\}^{T} = \left\{ \varepsilon^{D}_{\Omega_{11}} \quad \varepsilon^{D}_{\Omega_{22}} \quad \varepsilon^{D}_{\Omega_{33}} \quad \varepsilon^{D}_{\Omega_{12}} \quad \varepsilon^{D}_{\Omega_{13}} \quad \varepsilon^{D}_{\Omega_{23}} \right\},
$$

(6. 42)

Since $\mathbf{\bar{\varepsilon}}^{D}_{\Omega}$ can be arbitrary, the inequalities of diagonal terms in $\left[\left\langle \mathbf{C}_{\Omega}^{D} \right\rangle \right]$ and $\left[\left\langle \mathbf{C}_{\Omega/4}^{D} \right\rangle \right]$ can be determined. Taking $\left\{ \mathbf{\bar{\varepsilon}}^{D}_{\Omega} \right\}^{T} = [1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0]$, we have

$$
\frac{\tilde{E}^{D}_{\Omega}(1-v^{D}_{\Omega})}{(1+v^{D}_{\Omega})(1-2v^{D}_{\Omega})} \leq \frac{\tilde{E}^{D}_{\Omega/4}(1-v^{D}_{\Omega/4})}{(1+v^{D}_{\Omega/4})(1-2v^{D}_{\Omega/4})}
$$

(6. 43)

Expressing the above inequality in terms of the equivalent Young’s modulus as follows
where \( \tilde{\nu}_0 \) is a referenced value of the Poisson's ratio that \(-1.0 < \tilde{\nu}_0 < 0.5\) and \( \tilde{E}_{\Omega/a}^{D} \) are the average equivalent Young's moduli over the domains of two different RVE sizes.

Taking \( \{\tilde{E}_{\Omega/a}^{D}\}^{T} = \{0\ 0\ 0\ 1\ 0\ 0\} \), one can find

\[
\left\langle \frac{2\tilde{E}_{\Omega/a}^{D}}{(1+\tilde{\nu}_\Omega^{D})} \right\rangle \leq \left\langle \frac{2\tilde{E}_{\Omega/a}^{D}}{(1+\tilde{\nu}_\Omega^{D})} \right\rangle, \text{ or } \left\langle \tilde{G}_{\Omega/a}^{D} \right\rangle \leq \left\langle \tilde{G}_{\Omega/a}^{D} \right\rangle \tag{6.45}
\]

Repeating the same procedures to perform the partitioning of the RVE, the hierarchy of the material moduli can be determined:

\[
\left\langle \tilde{E}_{\Omega/a}^{D} \right\rangle \leq \left\langle \tilde{E}_{\Omega/a}^{D} \right\rangle \leq \cdots \leq \left\langle \tilde{E}_{\Omega/a}^{D} \right\rangle \tag{6.46}
\]

and

\[
\left\langle \tilde{G}_{\Omega/a}^{D} \right\rangle \leq \left\langle \tilde{G}_{\Omega/a}^{D} \right\rangle \leq \cdots \leq \left\langle \tilde{G}_{\Omega/a}^{D} \right\rangle \tag{6.47}
\]

The purpose for deriving the inequalities is to determine the size of the micro-structure which is sufficiently large. As the micro-structure size is large enough, the average value of the material moduli will converge. For the isotropic material, the two unknowns, i.e. \( \left\langle \tilde{E}_{\Omega}^{RVE} \right\rangle \) and \( \left\langle \tilde{G}_{\Omega}^{RVE} \right\rangle \), can be determined, as \( \left\langle \tilde{E}_{\Omega/a}^{D} \right\rangle \) and \( \left\langle \tilde{G}_{\Omega/a}^{D} \right\rangle \) converge.

Similar derivation can be made for the case with the Neumann boundary condition. The relationship between the averaged strain and stress is written as:
where $\tilde{\mathbf{S}}^N_\Omega$ is the effective compliance tensor under the Neumann boundary condition.

By substituting (6.48) into (6.22), the internal energy density can be rewritten as:

$$U = \frac{1}{2} \mathbf{\tilde{G}}^N_\Omega : \mathbf{\tilde{S}}^N_\Omega : \mathbf{\tilde{\sigma}}^N_\Omega$$  \hspace{1cm} (6.49)$$

Imposing the consistent Neumann boundary condition to the four sub-domains:

$$t^{N}_{\Omega_{ia}} = \sigma_{0} \cdot \mathbf{n} \quad \forall \mathbf{x} \in \partial \Omega_{ia}^\text{sub}, \ i=1, \ldots, 4$$  \hspace{1cm} (6.50)$$

The solution fields of the sub-domains are denoted as $\mathbf{u}^N_{\Omega_{ia}}$, $\mathbf{\sigma}^N_{\Omega_{ia}}$, and $\mathbf{\varepsilon}^N_{\Omega_{ia}}$, which should also be kinematically admissible. In this case, the averaged stresses of the sub-domains are the same as the overall averaged stress:

$$\mathbf{\tilde{\sigma}}^N_{\Omega_{ia}} = \sigma_{0} = \mathbf{\tilde{\sigma}}^N_\Omega$$  \hspace{1cm} (6.51)$$

For this case, the principle of the minimum total potential energy can also be applied:

$$\frac{1}{V} \left( \frac{1}{2} \int_{\Omega} \mathbf{\sigma}^N_\Omega : \mathbf{S} : \mathbf{\sigma}^N_\Omega \ d\Omega - \int_{\partial \Omega} t^N_{\Omega} \cdot \mathbf{u}^N_{\Omega} \ d\Gamma \right) \leq$$

$$\frac{1}{V} \sum_{i=1}^{4} \left( \frac{1}{2} \int_{\Omega_{ia}} \mathbf{\sigma}^N_{\Omega_{ia}} : \mathbf{S} : \mathbf{\sigma}^N_{\Omega_{ia}} \ d\Omega - \int_{\partial \Omega_{ia}} t^N_{\Omega_{ia}} \cdot \mathbf{u}^N_{\Omega_{ia}} \ d\Gamma \right)$$  \hspace{1cm} (6.52)$$

Similar to the case under the Dirichlet boundary condition, the displacement field $\mathbf{u}^N_{\Omega}$ and surface traction $t^N_{\Omega_{ia}}$ are continuous across the boundary of any two neighboring sub-domains, and $t^N_{\Omega} = t^N_{\Omega_{ia}}$ on the boundary of the overall domain, such that:

$$\int_{\partial \Omega} t^N_{\Omega} \cdot \mathbf{u}^N_{\Omega} \ d\Gamma = \sum_{i=1}^{4} \int_{\partial \Omega_{ia}} t^N_{\Omega_{ia}} \cdot \mathbf{u}^N_{\Omega_{ia}} \ d\Gamma$$  \hspace{1cm} (6.53)$$

Substituting (6.53) into (6.52), and applying the same concept of ergodicity, we have:

$$\mathbf{\tilde{\sigma}}^N_\Omega \leq \frac{1}{4} \sum_{i=1}^{4} \mathbf{\tilde{\sigma}}^N_{\Omega_{ia}} \cdot \frac{1}{2} \mathbf{\tilde{\sigma}}^N_\Omega : \mathbf{\tilde{S}}^N_\Omega : \mathbf{\tilde{\sigma}}^N_\Omega \leq \frac{1}{2} : \mathbf{\tilde{\sigma}}^N_\Omega : \mathbf{\tilde{S}}^N_\Omega : \mathbf{\tilde{\sigma}}^N_\Omega$$  \hspace{1cm} (6.54)$$
For an isotropic material, the inequality can be expressed in the following form:

\[
\frac{1}{2} \{ \bar{\sigma}^N_\Omega \}^T \left[ \begin{array}{c}
\left\langle S^N_\Omega \right\rangle \\
\left\langle A^N_\Omega \right\rangle \\
\left\langle B^N_\Omega \right\rangle 
\end{array} \right] \leq \frac{1}{2} \{ \bar{\sigma}^N_\Omega \}^T \left[ \begin{array}{c}
\left\langle S^N_{\Omega/4} \right\rangle \\
\left\langle A^N_{\Omega/4} \right\rangle \\
\left\langle B^N_{\Omega/4} \right\rangle 
\end{array} \right] \bar{\sigma}^N_\Omega
\]  
(6.55)

where

\[
\left\langle S^N_\Omega \right\rangle = \left[ \begin{array}{c}
\left\langle A^N_\Omega \right\rangle \\
\left\langle B^N_\Omega \right\rangle 
\end{array} \right],
\]

\[
\left\langle A^N_\Omega \right\rangle = \frac{1}{E^N_\Omega} \begin{bmatrix}
-\bar{\nu}^N_\Omega & 0 & 0 \\
0 & 1 & -\bar{\nu}^N_\Omega \\
0 & -\bar{\nu}^N_\Omega & 1
\end{bmatrix},
\]  
(6.56)

\[
\left\langle B^N_\Omega \right\rangle = \frac{2(1+\bar{\nu}^N_\Omega)}{E^N_\Omega} \begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{bmatrix}
\]

For the smaller microscopic cells, we have:

\[
\left\langle S^N_{\Omega/4} \right\rangle = \left[ \begin{array}{c}
\left\langle A^N_{\Omega/4} \right\rangle \\
\left\langle B^N_{\Omega/4} \right\rangle 
\end{array} \right],
\]

\[
\left\langle A^N_{\Omega/4} \right\rangle = \frac{1}{E^N_{\Omega/4}} \begin{bmatrix}
-\bar{\nu}^N_{\Omega/4} & 0 & 0 \\
0 & 1 & -\bar{\nu}^N_{\Omega/4} \\
0 & -\bar{\nu}^N_{\Omega/4} & 1
\end{bmatrix},
\]  
(6.57)

\[
\left\langle B^N_{\Omega/4} \right\rangle = \frac{2(1+\bar{\nu}^N_{\Omega/4})}{E^N_{\Omega/4}} \begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{bmatrix}
\]

and

\[
\{ \bar{\sigma}^N_\Omega \}^T = \{ \bar{\sigma}^N_{\Omega 11} \bar{\sigma}^N_{\Omega 22} \bar{\sigma}^N_{\Omega 33} \bar{\sigma}^N_{\Omega 12} \bar{\sigma}^N_{\Omega 23} \bar{\sigma}^N_{\Omega 31} \}.
\]  
(6.58)

Since \( \bar{\sigma}^N_\Omega \) can be arbitrary, the inequalities of diagonal terms in \( \left\langle S^N_\Omega \right\rangle \) and \( \left\langle S^N_{\Omega/4} \right\rangle \) can be determined. Taking \( \{ \bar{\sigma}^N_\Omega \}^T = \{ 1 \ 0 \ 0 \ 0 \ 0 \ 0 \} \) and \( \{ \bar{\sigma}^N_\Omega \}^T = \{ 0 \ 0 \ 0 \ 1 \ 0 \ 0 \} \), we have
Note that here the equivalent material moduli $\langle E^N_{\Omega} \rangle_{eq}$ and $\langle G^N_{\Omega} \rangle_{eq}$ will eventually converge to the effective moduli of the SRVE as a sufficiently large size of the microscopic cell is used, since the ensemble average will eventually converge to a constant when the field possesses ergodic properties. The hierarchy of the material moduli can be obtained for the case with the Neumann boundary condition:

$$\langle E^N_{\Omega\text{-iso}} \rangle_{eq} \leq \cdots \leq \langle E^N_{\Omega\text{-iso}} \rangle_{eq} \leq \langle E^N_{\Omega} \rangle_{eq}$$

(6. 61)

and

$$\langle G^N_{\Omega\text{-iso}} \rangle_{eq} \cdots \leq \langle G^N_{\Omega\text{-iso}} \rangle_{eq} \leq \langle G^N_{\Omega} \rangle_{eq}$$

(6. 62)

According to Hill’s definition, the overall effective moduli of the SRVE should be independent of the surface values of traction and displacement. As the SRVE is sufficiently large, the same averaged effective material moduli should be obtained under either the Dirichlet or the Neumann boundary condition. The hierarchy with respect to the microscopic cell size of the averaged effective material moduli then can be determined:

$$\langle E^N_{\Omega\text{-iso}} \rangle_{eq} \leq \cdots \leq \langle E^N_{\Omega\text{-iso}} \rangle_{eq} \leq \langle E^{\text{RVE}}_{\Omega} \rangle \leftarrow \langle E^D_{\Omega} \rangle_{eq} \leq \langle E^D_{\Omega\text{-iso}} \rangle_{eq} \leq \cdots \leq \langle E^D_{\Omega\text{-iso}} \rangle_{eq}$$

(6. 63)

and
Details for more general material laws can be found in the literature [91-93] and a more rigorous proof using techniques of homogenization and probability theories was given by Sab [125]. Note that if the micro-scale material moduli $C$ is an isotropic random field, $\tilde{C}_{RVE}^{\text{iso}}$ should become an isotropic tensor involving two Lamé constants $\tilde{\lambda}^{RVE}$ and $\tilde{\mu}^{RVE}$ [126]. Analogously, for an orthotropic random field $C$, $\tilde{\tilde{C}}^{RVE}$ should become an orthotropic tensor. In practice, the upper and lower bounds of the material moduli can help to determine the appropriate size of the microscopic cell which can be defined as the SRVE. As illustrated in Figure 6.3, when the microscopic cell size increases, the difference between the bounds of different boundary conditions decreases.

\[
\langle \tilde{G}^D \rangle \leq \langle \tilde{G}^N \rangle \rightarrow \langle \tilde{G}^{RVE} \rangle \leftarrow \langle \tilde{G}^R \rangle \leq \langle \tilde{G}_{\Omega/4}^D \rangle \leq \cdots \leq \langle \tilde{G}_{\Omega/\infty}^D \rangle \quad (6.64)
\]

Figure 6.3 Illustration for meso-scale bounds of material moduli

When the difference between the two bounds is sufficiently small that can be neglected, we can say that the given micro-structure is sufficiently large so the RVE is statistically representative for the entire micro-structure. Furthermore, as the size of RVE approach to infinite under the same pure boundary conditions and the microstructure possesses ergodicity, we have

\[
\lim_{\Omega \rightarrow \infty} \tilde{\sigma}_\Theta (\theta) = \lim_{\Omega \rightarrow \infty} \langle \sigma_\Omega (x) \rangle
\]

(6.65)
Note that the spatially averaged stress tensor \( \bar{\sigma}_\Omega (\theta) \) is still a function of \( \theta \) and \( \{\sigma_\Omega (x)\} \) is a function of \( x \). The ergodicity leads to the result that the two stress fields containing different variables in (6.65) should be constants:

\[
\lim_{\Omega \to \infty} \bar{\sigma}_\Omega (\theta) = \lim_{\Omega \to \infty} \{\sigma_\Omega (x)\} = \text{Constant} \tag{6.66}
\]

Under the pure Dirichlet boundary condition, the stress field can be expressed as the linear combination of homogenized material moduli and averaged strain:

\[
\bar{\sigma}_\Omega (\theta) = \tilde{C}_\Omega (\theta) : \bar{\varepsilon} \tag{6.67}
\]

Note that under the pure Dirichlet boundary condition, \( \bar{\varepsilon} \) is independent of random variable \( \theta \). With the condition (6.66), we conclude that when the RVE size is infinitely large, the material moduli approach constants:

\[
\lim_{\Omega \to \infty} \tilde{C}_\Omega (\theta) = \lim_{\Omega \to \infty} \{\tilde{C}_\Omega \} = \text{Constants} \tag{6.68}
\]

The above equation implies that when the RVE size is infinitely large, the homogenized material moduli becomes deterministic. Figure 6.4 shows the effect of increasing microscopic cell size on the deviation of stochastic material. When the microscopic cell size increases, the standard deviation of the material moduli approaches zero, indicating that the stochastic RVE eventually becomes the deterministic RVE.

Figure 6.4 Standard deviation vs. RVE size
(STD stands for standard deviation)
6.2 Size Effect of the Micro-crack Informed Multi-scale Damage Model

The objective of the dissertation is to develop a multi-scale damage model for brittle materials, such as concrete. In this section, we introduce the conventional homogenization methods to link the material behaviors between two different scales. The material failure observed in the macro-scale is regarded as the consequence of the crack formation and coalescence in the micro-scale. The macro-scale damage evolution is derived based on the loss the energy caused by crack initiation and propagation in the micro-scale via energy bridging method proposed by Ren and Chen et al. [82]. We will further discuss the size effect of the micro-crack informed multi-scale damage model. The size effect will then be proven by utilizing the principle of minimum total potential energy.

Consider a boundary value problem:

\[ \nabla \cdot \sigma = 0 \quad \text{in } \Omega \]  (6.69)

with the following boundary conditions:

\[ \sigma \cdot n = t \quad \text{on } \Gamma_t, \]
\[ \sigma \cdot n = h \quad \text{on } \Gamma_c, \]
\[ u = \bar{u} \quad \text{on } \Gamma_u \]  (6.70)

where \( \sigma \) is the total stress tensor, \( u \) is the total displacement field, \( t \) is the external traction acting on the boundary \( \Gamma_t \), \( h \) is the internal traction acting on the internal traction surface (crack surface) \( \Gamma_c \), \( \bar{u} \) is the prescribed boundary displacement. The total solution contains the coarse and fine scale responses. For a given material point in the macroscopic body, there is a corresponding micro-structural cell with domain \( \Omega \), containing heterogeneous constituents as well as cracks as shown in Figure 6.5.
The corresponding variational formation of (6.69) can be expressed as:

$$\int_\Omega \sigma : \delta \varepsilon \, d\Omega = \int_{\Gamma_t} t \cdot \delta u \, d\Gamma + \int_{\Gamma_h} h \cdot \delta u \, d\Gamma$$  \hspace{1cm} \text{(6. 71)}$$

where \( \varepsilon \) is the total strain field defined as:

$$\varepsilon = \frac{1}{2} \left( \nabla \otimes u + u \otimes \nabla \right)$$  \hspace{1cm} \text{(6. 72)}$$

and here a linear material law is considered:

$$\sigma = C : \varepsilon$$  \hspace{1cm} \text{(6. 73)}$$

Directly solving the equations (6.69)–(6.70) of a large system regarding the microscopic defects and heterogeneities is computationally expensive. The purpose of this research is to establish the homogenization process as shown in Figure 6.6 for materials with defects.

The tractions and displacements prescribed on the outer boundary of the microscopic cell.
\( \partial \Omega \) are related to the homogenized stress and strain in the continuum as:

\[
\tilde{\sigma}_{\Omega} = \frac{1}{V_y} \int_{\partial \Omega} t_{\Omega} \otimes x \, d\Gamma = \frac{1}{V_y} \int_{\partial \Omega} \sigma_{\Omega} \cdot n \otimes x \, d\Gamma
\]

(6.74)

\[
\tilde{\varepsilon}_{\Omega} = \frac{1}{2V_y} \int_{\partial \Omega} \left( u_{\Omega} \otimes n + n \otimes u_{\Omega} \right) \, d\Gamma
\]

(6.75)

where the quantities with subscript \( \Omega \) are the fields in the domain \( \Omega \), the tilde "~" denotes the homogenized quantities and \( V_y \) is the volume of the base cell.

Recall the definition of the spatially averaged stress and stress tensors from (6.4) and (6.20):

\[
\bar{\sigma}_{\Omega} = \frac{1}{V_y} \int_{\Omega} \sigma_{\Omega} \, d\Omega
\]

(6.76)

\[
\bar{\varepsilon}_{\Omega} = \frac{1}{V_y} \int_{\Omega} \varepsilon_{\Omega} \, d\Omega
\]

(6.77)

The relationship between the homogenized and spatially averaged stresses for materials with internal cracks can then be easily derived:

\[
\bar{\sigma}_{\Omega} = \frac{1}{V_y} \int_{\Omega} \sigma_{\Omega} \, d\Omega = \frac{1}{V_y} \int_{\Omega} \nabla \left( \sigma_{\Omega} \otimes x \right) \, d\Omega
\]

\[
= \frac{1}{V_y} \int_{\partial \Omega} \left( \sigma_{\Omega} \cdot n \otimes x \right) \, d\Gamma - \frac{1}{V_y} \int_{\Gamma} \left( \sigma_{\Omega} \cdot n \otimes x \right) \, d\Gamma
\]

(6.78)

\[
= \sigma_{\Omega} - \frac{1}{V_y} \int_{\Gamma} \left( h_{\Omega} \otimes x \right) \, d\Gamma
\]

Note that the second term in the right hand side of the above equation vanishes due to the imposition the self-equilibrated cohesive traction \( h_{\Omega} \) on the crack surface. Hence,

\[
\bar{\sigma}_{\Omega} = \tilde{\sigma}_{\Omega}
\]

(6.79)

On the other hand, the relationship between the spatially averaged strains and the spatially homogenized strains for materials with internal cracks is:
If the micro-structure contains voids or micro-cracks the second term in the right hand side of the above equation won't vanish, since there exists displacement jumps across the crack surfaces or voids. Consequently, the homogenized strain cannot be represented by the spatially averaged strain.

Next, we introduce the Helmholtz free energy (HFE) \( \Psi_\Omega \) to describe macro-scale material failure caused by the growth and coalescence of micro-cracks. The HFE is defined as the product of homogenized stress and strain tensors:

\[
\bar{\Psi}_\Omega = \frac{1}{2} \bar{\sigma}_\Omega : \bar{\varepsilon}_\Omega 
\]  \hspace{1cm} (6. 81)

and:

\[
\bar{\sigma}_\Omega = \frac{\partial \bar{\Psi}_\Omega}{\partial \bar{\varepsilon}_\Omega} \hspace{1cm} (6. 82)
\]

On the other hand, the microscopic free energy is defined as:

\[
\Psi_\Omega = \frac{1}{2} \sigma_\Omega : \varepsilon_\Omega \hspace{1cm} (6. 83)
\]

Integrating the microscopic free energy over the microscopic domain \( \Omega \), and applying the condition of vanishing body force, we have:

\[
\int_{\Omega} \Psi_\Omega \, d\Omega = \int_{\Omega} \frac{1}{2} \sigma_\Omega : \varepsilon_\Omega \, d\Omega = \int_{\Omega} \frac{1}{2} \sigma_\Omega : \frac{1}{2} \left( \nabla \otimes u_\Omega + u_\Omega \otimes \nabla \right) d\Omega \\
= \int_{\Omega} \frac{1}{2} \nabla \cdot \left( u_\Omega \otimes \sigma_\Omega \right) d\Omega \hspace{1cm} (6. 84)
\]

then introducing the divergence theorem to the above equation, microscopic free energy can be expressed as:
We impose pure Dirichlet boundary conditions in the microscopic cell, where the boundary displacement field is given in the form of (6.3):

$$u_{\Omega_0}^D = \bar{u}_{\Omega_0}^D \cdot x \quad \text{on} \quad \partial \Omega,$$

(6.86)

Substituting (6.86) into the first term on the right hand side of (6.85), we have:

$$\int_{\Omega_0} \Psi_{\Omega_0}^D d\Omega = \int_{\Omega_0} \frac{1}{2} \mathbf{t}_{\Omega_0}^D \cdot \left( \mathbf{e}_{\Omega_0}^D \cdot x \right) d\Omega - \int_{\Gamma_2} \frac{1}{2} \mathbf{h}_{\Omega_0}^D \cdot \mathbf{u}_{\Omega_0}^D d\Gamma$$

$$= \int_{\Omega_0} \frac{1}{2} \mathbf{t}_{\Omega_0}^D \cdot \mathbf{x} d\Omega - \int_{\Gamma_2} \frac{1}{2} \mathbf{h}_{\Omega_0}^D \cdot \mathbf{u}_{\Omega_0}^D d\Gamma$$

(6.87)

Rearranging (6.87), the relationship between the Helmholtz free energy of the homogenized continuum and the microscopic free energy can be obtained through energy bridging:

$$\Psi_{\Omega_0}^D = \frac{1}{V_y} \left( \int_{\Omega_0} \Psi_{\Omega_0}^D d\Omega + \int_{\Gamma_2} \frac{1}{2} \mathbf{h}_{\Omega_0}^D \cdot \mathbf{u}_{\Omega_0}^D d\Gamma \right)$$

(6.88)

Once the Helmholtz free energy of the homogenized continuum is obtained, the damage evolution can be determined through the calculation of energy dissipation. Hence, the damage model of the homogenized continuum can be expressed as:

$$\Psi_{\Omega_0}^D = (1 - d_{\Omega_0}^D) \Psi_{0, \Omega_0}^D$$

(6.89)

where $d_{\Omega_0}^D$ is the damage parameter and $\Psi_{0, \Omega_0}^D$ is the effective Helmholtz free energy of the undamaged homogenized continuum:

$$\Psi_{0, \Omega_0}^D = \frac{1}{2} \mathbf{e}_{\Omega_0}^D : \mathbf{\bar{e}}_{0, \Omega_0}^D : \mathbf{\bar{e}}_{\Omega_0}^D$$

(6.90)

Similar to the previous section, to discuss the size effect for the multi-scale damage modeling, we introduce the principle of minimum total potential energy with cohesive
micro-cracks again. Modifying the positive functional \( F(\mathbf{u}, \hat{\mathbf{u}}) \) in (6.29) with the consideration of internal cracks, we have:

\[
F(\mathbf{u}, \hat{\mathbf{u}}) = \frac{1}{2} \int_{\Omega} (\varepsilon - \hat{\varepsilon}) : \mathbf{C} : (\varepsilon - \hat{\varepsilon}) \, d\Omega + \frac{1}{2} \int_{\Gamma_c} \left( [\mathbf{u}] - [\hat{\mathbf{u}}] \right) \left( k'([\mathbf{u}] - [\hat{\mathbf{u}}]) \right) \, dS \geq 0 \quad (6.91)
\]

where \([\mathbf{u}]\) and \([\hat{\mathbf{u}}]\) are displacement jumps across the crack surface, \(l_c\) is the length of fracture process zone, \(k' (\geq 0)\) is the coefficient of cohesive law, i.e. \(k' = f_s/[\mathbf{u}] - k\) for linear cohesive law, in which \(f_s\) the material tensile strength and \(k\) is a constant denoting the slope of the cohesive law.

Expanding (6.91), the principle of minimum total potential energy can be derived:

\[
\frac{1}{2} \int_{\Omega} \mathbf{\sigma} : \varepsilon d\Omega + \frac{1}{2} \int_{\Gamma_c} [\mathbf{u}] k' \, ds - \int_{\partial \Omega} \mathbf{u} \cdot t \, d\Gamma \leq \frac{1}{2} \int_{\Omega_c} \mathbf{\hat{\sigma}} : \hat{\varepsilon} d\Omega + \frac{1}{2} \int_{\Gamma_c} [\hat{\mathbf{u}}] k' \, ds - \int_{\partial \Omega} \hat{\mathbf{u}} \cdot t \, d\Gamma \quad (6.92)
\]

Performing the partitioning technique again as aforementioned, and replacing the perturbation terms by the sub-domain fields \(\mathbf{u}^D_{\Omega_i}\) and \(\mathbf{\varepsilon}^D_{\Omega_i}\), which are kinematically admissible, we have:

\[
\frac{1}{V_i} \left( \int_{V_i} \Psi^D_{\Omega_i} \, d\Omega + \frac{1}{2} \int_{\Gamma_i} \mathbf{u}^D_{\Omega_i} \cdot \mathbf{h}^D_{\Omega_i} \, ds - \int_{\partial \Omega_i} \mathbf{u}^D_{\Omega_i} \cdot \mathbf{t}^D_{\Omega_i} \, d\Gamma \right) \leq \frac{1}{V_i} \sum_{i=1}^{4} \left( \int_{V_i} \Psi^D_{\Omega_i} \, d\Omega + \frac{1}{2} \int_{\Gamma_i} \mathbf{u}^D_{\Omega_i} \cdot \mathbf{h}^D_{\Omega_i} \, ds - \int_{\partial \Omega_i} \mathbf{u}^D_{\Omega_i} \cdot \mathbf{t}^D_{\Omega_i} \, d\Gamma \right) \quad (6.93)
\]

Note the following conditions have been applied to the above inequality:

\[
\frac{1}{2} \int_{\Gamma_c} [\mathbf{u}] k' \, ds = \int_{\Gamma_c} \mathbf{u} \cdot \mathbf{h} \, ds \quad (6.94)
\]

Since the displacement field \(\mathbf{u}^D_{\Omega_i}\) and surface traction \(\mathbf{t}^D_{\Omega_i}\) are continuous across the boundary of any two neighboring sub-domains under the pure Dirichlet boundary condition, and \(\mathbf{u}^D_{\Omega_i} = \mathbf{u}^D_{\Omega_j}\) on the overall boundary of the entire domain, (6.33) holds. Thus, we can
deduce from (6.93) to the following form:

\[
\frac{1}{V} \left( \int_{\Omega_y} \Psi^{D}_{\Omega_y} \, d\Omega + \frac{1}{2} \int_{\Omega_y} \mathbf{u}^{D}_{\Omega_y} \cdot \mathbf{h}^{D}_{\Omega_y} \, ds \right) \leq \frac{1}{V} \sum_{i=1}^{4} \left( \mathbf{d}_{\Omega_i}^{D} \right) \Psi^{D}_{\Omega_i} \, d\Omega + \frac{1}{2} \int_{\Gamma} \mathbf{u}^{D}_{\Omega_i} \cdot \mathbf{h}^{D}_{\Omega_i} \, ds \quad (6.95)
\]

Using the relationship among the Helmholtz free energy of the homogenized continuum, the microscopic free energy and cohesive energy in (6.88), eventually we obtain the following inequality in terms of the Helmholtz free energy, namely:

\[
\mathbf{d}_{\Omega_i}^{D} \leq \frac{1}{4} \sum_{i=1}^{4} \mathbf{d}_{\Omega_i}^{D} 
\]

(6.96)

With ergodicity, we have:

\[
\left\langle \mathbf{d}_{\Omega_i}^{D} \right\rangle \leq \left\langle \mathbf{d}_{\Omega_i}^{D} \right\rangle 
\]

(6.97)

Applying (6.89) to (6.97), it yields:

\[
\left\langle \left( 1 - \mathbf{d}_{\Omega_i}^{D} \right) \mathbf{d}_{\Omega_i}^{D} \right\rangle \leq \left\langle \left( 1 - \mathbf{d}_{\Omega_i}^{D} \right) \mathbf{d}_{\Omega_i}^{D} \right\rangle 
\]

(6.98)

Furthermore, assume the microscopic cell size is sufficiently large such that the undamaged material moduli approach a constant:

\[
\mathbf{d}_{\Omega_i}^{D} = \mathbf{d}_{\Omega_i}^{D} = \frac{1}{2} \mathbf{e}^{D}_{\Omega_i} : \mathbf{C}^{D}_{0-\Omega_i} : \mathbf{e}^{D}_{\Omega_i} 
\]

(6.99)

We then obtain:

\[
\left\langle \mathbf{d}_{\Omega_i}^{D} \right\rangle \geq \left\langle \mathbf{d}_{\Omega_i}^{D} \right\rangle 
\]

(6.100)

Following the same procedures of partitioning the RVEs, the hierarchy of the damage parameter can be obtained:

\[
\left\langle \mathbf{d}_{\Omega_i}^{D} \right\rangle \geq \left\langle \mathbf{d}_{\Omega_i}^{D} \right\rangle \geq \ldots \geq \left\langle \mathbf{d}_{\Omega_i}^{D} \right\rangle 
\]

(6.101)

The above inequalities agree with the phenomenological Weibull-type representation of brittle solids: the larger the specimen the more likely it is to fail. With fixed characteristic length of the structure, e.g. employing the same cohesive law regardless the structural dimension, a larger structure fails easier.

Now, consider the deterministic case: a micro-structure containing micro-cracks purely
As the micro-structure is periodic, we can modify (6.96) as:

\[
\tilde{\Psi}_y^{\Omega_y} \leq \tilde{\Psi}_y^{\Omega_y/4}, \quad \text{since} \quad \tilde{\Psi}_y^{\Omega_y} = \tilde{\Psi}_y^{\Omega_y/4}
\]  

(6. 102)

As illustrated in Figure 6.8, the total HFE of the sub-domains is equal to the twicely enlarged micro-structure where the total energy is expressed as follows:

\[
4 \left( \frac{1}{4} V_y \right) \tilde{\Psi}_y^{\Omega_y/4} = V_y \tilde{\Psi}_y^{\Omega_y/4} = V_y \tilde{\Psi}_y^{\Omega_y/4}
\]  

(6. 103)

in which \( V_y \tilde{\Psi}_y^{\Omega_y/4} \) denotes the energy of the enlarged micro-structure with a single crack which is also proportionally enlarged as plotted in the right-hand side of Figure 6.8. Substituting (6.103) into (6.102), the structure with a single crack has larger energy than the one with 4 smaller cracks. In the finite element analysis, if damage evolution is not scaled with the RVE size, the refinement actually changes the characteristic length of RVE at macroscale. Hence the case with a single larger crack can be regarded as a model with the coarse discretization. Here, superscript 'Coarse' is used to denote the coarse discretization in the domain \( \Omega_y \). Repeating the same procedures, the inequalities between different discretizations can be obtained:

\[
V_y \tilde{\Psi}_y^{\Omega_y/4} \geq \cdots \geq V_y \tilde{\Psi}_y^{\Omega_y/4}
\]  

(6. 104)
The above inequalities mean that a numerical model with the finer discretization contains smaller energy than the one with the coarser discretization. If the RVE size is not consistent with the mesh size, the numerical results do not converge along with the mesh refinement when the material enters the softening region as illustrated in Figure 6.10. Such phenomenon is called mesh dependency. To remedy the mesh dependency, some approaches such as non-local theories were introduced to the finite element models [127-129] or in mesh-free methods the non-locality is embedded in the kernel function (or weight function) [130-131], such that the numerical results are mesh insensitive. In the next section, an approach to remedy the size effect will be discussed.

\[
V_y \tilde{\Psi}_{\Omega_i} \leq 4 \left( \frac{1}{4} V_y \right) \tilde{\Psi}_{\Omega_i/4} \leq V_y \tilde{\Psi}_{\Omega_i}^{D, \text{Coarse}}
\]

Figure 6.8 Illustration of the size effect of periodic micro-structures

\[
V_y \tilde{\Psi}_{\Omega_i}^{D, \text{Fine}} \leq \cdots \leq V_y \tilde{\Psi}_{\Omega_i}^{D, \text{Coarse}}
\]

Figure 6.9 Size effect of model refinement
6.3 A Remedy for Size Effect

As discussed in the previous section, the solution of a problem with material degradation exhibits size effect if the characteristic length is not defined to be independent to the mesh size. Here we conduct a set of numerical simulations for different micro-geometries of a ultra-high strength concrete and calculate the averaged load-displacement curves. Three different microscopic cell sizes, 5x5 mm$^2$, 2.5x2.5 mm$^2$ and 1.25x1.25 mm$^2$, are used to conduct the convergence study. Several samples of the microstructure are shown in Figure 6.11. A simplified 2-phase model, voids and matrix, is used for the numerical simulations. More details of the concrete properties will be discussed in Chapter 7.

The homogenized stress and strain curves under the uni-axial tension are plotted in
Figure 6.12. The corresponding damage evolution curves are plotted in Figure 6.13. The y-axis in Figure 6.12 is the microscopic cell size normalized by the dimension of the macro-structure as shown in Figure 6.14, which is $L = 0.1$ m. With the damage evolution curves obtained by using the energy bridging method, macro-scale numerical simulations can be conducted. Consider a notched beam subjected to a load on the top of the mid-span as shown in Figure 6.14. The overall behavior of the beam is governed by the Mode I crack initiated at the vertex of the notch. In this example, we consider that the damage evolution is driven by the tensile damage only due to the bending condition and the substantial strength in compression of the concrete. The material properties of the Young's modulus and Poisson's ratio are 21.5 GPa and 0.22, respectively. For this problem, only half of the beam is modeled for numerical simulations due to the symmetric conditions.

![Figure 6.12 Average homogenized stress-strain curves of different RVE sizes](image)

Figure 6.12 Average homogenized stress-strain curves of different RVE sizes

![Figure 6.13 Average damage evolution curves of different RVE sizes](image)

Figure 6.13 Average damage evolution curves of different RVE sizes
In this work, various sizes of microscopic cells corresponding to macro-structural discretizations with coarse, medium and fine meshes are considered to study the size effect. For this purpose, a dimensionless parameter, $\lambda$, is defined as follows:

$$\lambda = \frac{l_{\text{mic}}}{l_{\text{mac}}} = \frac{l}{L}$$  \hspace{1cm} (6. 105)

where $l_{\text{mic}}$ is the microscopic length parameter and $l_{\text{mac}}$ is the macroscopic length parameter. Here we chose the microscopic cell size $l=5$ mm, 2.5 mm and 1.25 mm as the microscopic length parameters and the beam depth $L$ as the macroscopic length parameter. Figure 6.15 demonstrates the size dependency of the calculated nominal strength which can be fitted to the size effect law proposed by Bazant [132]:

$$\sigma_{N} = \frac{B f_{u}}{\sqrt{1 + \beta}}, \hspace{0.5cm} \beta = \frac{l}{l_{0}}$$  \hspace{1cm} (6. 106)

where $f_{u}$ is the tensile strength of concrete, $l$ is the specimen dimension, and $B$ and $l_{0}$ are material parameters identified by experiments or numerical simulation.

![Figure 6.15 The size effect curve of nominal strength](image)
The size dependency is due to the influence of the internal length scale, i.e., the void size and the cohesive crack law do not scale with the overall dimensions of the microscopic cells. Consequently, the various nominal strength values are obtained through different sizes of the microscopic cells. As being pointed out in the previous section, if the discretization is refined without considering the relationship between microstructure dimension and mesh size, the solutions exhibit mesh dependency. Figure 6.16 shows a strong mesh dependency induced by the standard procedure in the conventional damage mechanics, where only one microscopic cell is used to characterize the damage evolution equation. Note the microscopic cell sizes for the coarse, medium and fine discretizations are 5 mm², 2.5 mm² and 1.25 mm², respectively, and the damage evolution law adopted is only the one with the microscopic cell size 5 mm². The microscopic cell size is only consistent with the coarse discretization but not with the medium and fine discretizations.

To resolve the problem of mesh dependency, an approximated damage evolution with a scaling law is introduced:

\[ d = \frac{\varepsilon - \varepsilon_i}{\varepsilon_u - \varepsilon_i}, \quad \varepsilon_i = \varepsilon_i(\lambda), \quad \varepsilon_u = \varepsilon_u(\lambda) \]  \hspace{1cm} (6.107)

where \( \varepsilon_i \) and \( \varepsilon_u \) are the damage initiation strain and the rupture strain, respectively. Both of the two parameters are functions of the dimensionless parameter \( \lambda \), which has been defined in (6.105). The damage initiation strain \( \varepsilon_i \) is assumed to be in a form similar to (6.106), which can be expressed as:

\[ \varepsilon_i = \frac{A}{\sqrt{1 + \alpha \lambda}} \]  \hspace{1cm} (6.108)

and \( (\varepsilon_u - \varepsilon_i) \) is assumed as (Ren and Chen et al., 2011):

\[ (\varepsilon_u - \varepsilon_i) = C \lambda^n \]  \hspace{1cm} (6.109)

where \( A, \alpha, C \) and \( n \) are constants which can be obtained by fitting the approximated damage evolution curves into the homogized damage evolution curves:
In this case, only three different RVE sizes are considered to determine the parameters in (6.110). The approximated damage evolution curves are plotted together with the homogenized damage evolution curves as shown in Figure 6.17. By introducing the damage evolution function with a scaling law, the mesh insensitive results can be obtained as shown in Figure 6.18. This approach avoids the need for RVE analyses with different dimensions that match the corresponding continuum scale mesh dimensions.

\[
A = 0.53336 \times 10^{-4}, \quad \alpha = 9.38776 \\
C = 0.48918 \times 10^{-4}, \quad n = -0.43116
\]  

(6.110)

Figure 6.16 Mesh dependent load–displacement responses using inconsistent sizes of the microscopic cells

Figure 6.17 Average approximated and homogenized damage evolution curves of different RVE sizes
Figure 6.18 Mesh independent load–displacement responses using the damage evolution function with a scaling law

6.4 A Two-parameter Damage Model

In this work, we introduce a two-parameter damage model containing the shear and volumetric failure modes:

\[ \Psi = (1 - d_{vol})\Psi_{0,\text{vol}} + (1 - d_{dev})\Psi_{0,\text{dev}} \]  

where \( d_{vol} \) and \( d_{dev} \) are the corresponding volumetric and deviatoric damage parameters and \( \Psi_{0,\text{vol}} \) and \( \Psi_{0,\text{dev}} \) are volumetric and deviatoric parts of the effective Helmholtz free energy.

The effective free energy can be expressed in terms of undamaged homogenized material moduli and homogenized stress and strain:

\[ \Psi_{0} = \frac{1}{2} \dot{\varepsilon} : \dot{\epsilon} = \frac{1}{2} \dot{\sigma} : \dot{\epsilon} \]

\[ = \Psi_{0,\text{vol}} + \Psi_{0,\text{dev}} \]  

\[ \Psi_{0,\text{vol}} = \frac{1}{2} \dot{\sigma}_{0,\text{vol}} : \dot{\epsilon} \]  

\[ \Psi_{0,\text{dev}} = \frac{1}{2} \dot{\sigma}_{0,\text{dev}} : \dot{\epsilon} \]

where
The Helmholtz free energy is decomposed into elastic and plastic parts:

\[
\tilde{\Psi}_{0_{\text{vol}}} = \frac{1}{3} tr(\tilde{\sigma}_0) \mathbf{1}, \\
\tilde{\Psi}_{0_{\text{dev}}} = \tilde{\sigma}_0 - \tilde{\sigma}_{0_{\text{vol}}} 
\]

\[ (6.114) \]

The proposed model assumes the damage evolution to be only related to the elastic Helmholtz free energy:

\[
\tilde{\Psi}_{0_{\text{vol}}} = \tilde{\Psi}_{0_{\text{vol}}}^e + \tilde{\Psi}_{0_{\text{vol}}}^p \\
\tilde{\Psi}_{0_{\text{vol}}}^e = (1 - d_{vol}) \tilde{\Psi}_{0_{\text{vol}}}^e + (1 - d_{dev}) \tilde{\Psi}_{0_{\text{dev}}}^e \\
\tilde{\Psi}_{0_{\text{vol}}}^p = (1 - d_{vol}) \tilde{\Psi}_{0_{\text{vol}}}^p + (1 - d_{dev}) \tilde{\Psi}_{0_{\text{dev}}}^p 
\]

\[ (6.115), (6.116), (6.117), (6.118) \]

where the superscript "e" denotes elastic and "p" denotes plastic.

In the proposed model, the damage evolution is assumed to be only related to the elastic Helmholtz free energy:

\[
d_{vol} = \left( 1 - \frac{\partial \tilde{\Psi}}{\partial \tilde{\Psi}_{0_{\text{vol}}}} \right) = \left( 1 - \frac{\partial \tilde{\Psi}^e}{\partial \tilde{\Psi}_{0_{\text{vol}}}^e} \right) \\
d_{dev} = \left( 1 - \frac{\partial \tilde{\Psi}}{\partial \tilde{\Psi}_{0_{\text{dev}}}} \right) = \left( 1 - \frac{\partial \tilde{\Psi}^e}{\partial \tilde{\Psi}_{0_{\text{dev}}}^e} \right) 
\]

\[ (6.119), (6.120) \]

The elastic Helmholtz free energy \( \tilde{\Psi}^e \) can be obtained through the homogenization process of (6.88) by imposing the pure shear and tensile boundary conditions. The shear damage mode can be determined by imposing pure shear case onto the micro-scale level as shown in Figure 6.19 (a):

\[
d_{dev} = \left( 1 - \frac{\tilde{\Psi}^e}{\tilde{\Psi}_{0_{\text{dev}}}^e} \right) 
\]

\[ (6.121) \]

In the proposed model, only bi-axial or uni-axial tensile numerical simulations can be conducted in the 2-D cohesive fracture model. The volumetric damage evolution will then be determined by imposing bi-axial or uni-axial tension on the micro-scale level:

\[
d_{vol} = \left( 1 - \frac{\tilde{\Psi}_{0_{\text{vol}}}^e}{\tilde{\Psi}_{0_{\text{vol}}}^e} \right) 
\]

\[ (6.122) \]
On the macroscopic level, a phenomenological constitutive model is introduced for the yield criterion of plasticity effect. The adopted phenomenological model is based on the advanced fundamental concrete (AFC) model [133-134], where the material behavior is based upon the separation of the hydrostatic and deviatoric behaviors. The yield surface of the AFC model is expressed in the following form if the first invariant of the stress tensor ($I_1$) is less than zero (indicative of compression):

$$F(\sigma_{dev}, I_1) = \left\| \sigma_{dev} \right\| - \left\{ C_1 - \left[ C_2 + (C_1 - C_2)D \right] e^{A_n I_1} - C_4 I_1 \right\} \left( 1 + C_3 \ln (\dot{\varepsilon}_n) \right)$$

(6.123)

where $F(\sigma_{dev}, I_1)$ is the function of yield surface, $C_1$, $C_2$, $C_3$ and $C_4$ and $A_n$ are constants that are greater than or equal to zero. It should also be noted that the values of $C_1$ and $C_2$ must satisfy the constraint $C_1 \geq C_2$. $D$ is the damage parameter that varies from 0 to 1 and $\dot{\varepsilon}_n$ is an effective deviatoric strain rate. This material damage model effectively provides a reduced failure surface due to excessive plastic shear strain as well as excessive hydrostatic pressure.

The damage evolution of the AFC model is expressed as:

$$D = \sum_{i=1}^{\sigma} \left[ \frac{\Delta \varepsilon_p}{-I_1 D_1} + \frac{\Delta \mu_p}{1.5U_{lock}} \right]$$

(6.124)

where $D_1$ is a parameter which is greater than zero, $\Delta \varepsilon_p$ and $\Delta \mu_p$ are the $i$-th increment of the effective deviatoric plastic strain, and the volumetric plastic strain, and
respectively, and $U_{lock}$ is the locking volumetric strain value, which is an input parameter
defining the volumetric strain value where the material locking occurs. In the AFC model, the
determination of the damage evolution $D$ is purely phenomenological, which is based on the
observation from experiments, while in our work, the damage evolution will be determined
through multi-scale modeling. The proposed stochastic multi-scale damage model employs
the plastic yield criterion of AFC model while its phenomenological damage law is replaced
by the multi-scale damage evolution. We consider a similar form of the AFC model in (6.123)
\[
F(\sigma_{dev}, I_1) = \|\sigma_{dev}\| - \left\{ \dot{C}_1^* + \left[ C_2^* + (C_3^* - C_4^*)d^* \right] e^{\lambda h} - C_4^* I_1 \right\} \left( 1 + C_3^* \ln (\dot{e}_n) \right)
\]  
(6.125)
where the parameters with superscript ‘*’ are assumed to be random functions. Note that a
different notation of the damage parameter “$d^*$” is used, since the damage evolution is
obtained from the multi-scale modeling. The random parameters $C_1^* \sim C_4^*$ are assumed as
the following form:
\[
C_i^* = C_i \left( 1 + \alpha_i \xi \right), \quad i = 1 \sim 4
\]
\[
d^* = d \left( 1 + \beta \xi \right)
\]  
(6.126)
where $\xi$ is a random variable and $\alpha_i$ and $\beta$ are constants corresponding to the parameter
$C_i^*$ and $d^*$. If $\xi$ is a random variable with zero mean and unit variance, $|\alpha_i|$ and $\beta$
will be the standard deviation of the parameter $C_i^*$ and $d^*$ normalized by their average. The
parameters $C_i$ and $d$ can be regarded as the mean values of $C_i^*$ and $d^*$ respectively.
More details of the parameter $C_i^*$ for the practical use will be discussed in Chapter 7. Here,
we slightly modify the AFC model, where a hardening law is introduced to the parameter
$\dot{C}_1^*$:
\[
\dot{C}_1^* = C_1^* \left( 1 + h \bar{\varepsilon}_p \right),
\]  
(6.127)
where $h$ is the hardening parameter, and $\bar{\varepsilon}_p$ is the effective plastic strain. The hardening law
is introduced to provide sufficient stiffness after the material yields. Here a two-stage hardening rules are adopted:

\[
\begin{align*}
&\begin{cases}
  h = h_a, & \text{at initial yield point} \\
  h = h_b, & \text{when } \|\sigma_{dev}\| = \sigma_d'(1 + \gamma) \\
\end{cases}
\end{align*}
\]  

(6.128)

where \(h_a\), \(h_b\) and \(\gamma\) are constants and \(\sigma_d\) is the damage initiation stress which is assumed to be a function of the first invariant of the stress tensor \((I_1)\):

\[
\sigma_d = a_1 + a_2 I_1 + a_3 I_1^2
\]

(6.129)

When \(\|\sigma_{dev}\|\) reaches the critical value, the parameter \(\hat{\dot{C}}_i\) becomes

\[
\hat{\dot{C}}_i = C_i'' \left(1 + h_b \bar{\varepsilon}_p\right), \quad C_i'' = C_i'(1 + h_a \bar{\varepsilon}^d_p)
\]

(6.130)

in which \(\bar{\varepsilon}^d_p\) is the effective plastic strain when \(\|\sigma_{dev}\| = \sigma_d\).

Figure 6.20 illustrates the characteristics of the yield criterion as \(I_1 < 0\). As can be seen in the figure, the initial yield stress is the difference between the constants \(C_1\) and \(C_2\). Beyond the initial yield point, the material hardening provides sufficient stiffness for the yield surface to grow. At some point, the damage is initiated and the hardening rule is changed. Note that the damage law is already embedded in the yield surface as shown in (6.125). The yield surface is the result under the coupling effect of the material failure and yielding.

![Figure 6.20 Modified yield surface of AFC model](image)
6.5 Summary

In this chapter, the characteristic length of the stochastic representative volume element (SRVE) is addressed. The existence of SRVE is demonstrated through the satisfaction of the Hill condition, ergodicity and the principle of the minimum potential energy, where the first two are assumptions and the last one is due to the nature of the continuum mechanics. For problems regarding the material degradation, the solutions exhibit size effect. The statistical damage mechanics stated that the larger the specimen the more likely it is to fail, which is consistent with the conclusion we made in the field of SRVE: the larger microscopic cell size is, the more likely the material fails. To remedy the mesh dependency in the numerical simulations, a damage evolution with a size scaling law is proposed. With the size scaled damage evolution, the mesh insensitive results can be obtained.

At last, a two-parameter multi-scale damage model is proposed, which considers the shear and volumetric failures. The failure modes in the proposed model is consistent with the phenomenological AFC model, where the material damage yields a reduced failure surface due to excessive plastic shear strain as well as excessive hydrostatic crushing. The proposed stochastic multi-scale damage model employs the plastic yield criterion of AFC model, while its phenomenological damage law is replaced by the multi-scale damage evolution. In the next chapter, numerical simulations will be performed for practical problems to validate the proposed stochastic multi-scale damage model.
Chapter 7

Applications

In this chapter, the aforementioned stochastic multi-scale modeling is applied to predicting responses of concrete subjected to tri-axial compression. The procedures of the multi-scale modeling are illustrated in Figure 7.1. The micro-structural geometry based on the computerized tomography (CT) scans is constructed and the fracture mechanics based numerical simulation of the micro-structural failure processes is then conducted. The fracture modeling techniques described in Chapter 5 are employed for the RVE analyses. The corresponding stress-strain curves are then obtained through the numerical analysis, and the Helmholtz free energy is consequently calculated based on the energy bridging method as shown in equation (6.88). Finally, the stochastic damage evolution function is extracted from the loss of Helmholtz free energy following (6.89).

Due to the heterogeneity of microstructure, the macro-scale damage parameter is considered as a random function which exhibits a noticeable uncertainty. The stochastic method described in Chapters 3 and 4 is introduced to evaluate the uncertainty for the investigated concrete materials.
7.1 The Characteristics of the Concrete Material Under Consideration

The material under consideration is an ultra-high strength concrete [135]. Several samples of the CT scans of the concrete are shown in Figure 7.2. The aggregates used in this concrete are silica sand. The shapes of the aggregates are irregular which provides a tight bond between the cement and the aggregates. The gradation for the aggregates used in the material is listed in Table 7.1, where the sieve size of No. 30 is 0.595 millimeters and 96% of the aggregates have a diameter smaller than 0.595 millimeters. The largest void diameter is roughly 0.6 millimeter, which is close to size of the largest aggregates. The concrete was under curing process for 91 days, which is sufficient for the cement to develop its strength. The water to cement ratio for the material was 0.40. This would be considered low for a self-consolidating concrete, but high for an ultra-high strength concrete so that the aggregates can be more uniformly distributed within the specimen.

Due to the characteristics of the material, the adopted numerical simulation model is simplified as a two phase material; the matrix and voids. The effects of aggregates and the
interface between aggregates and the cement are neglected, since the irregularity of the aggregate shape is high which provides an appropriate bonding of the interface. Also, the uniformity of the aggregate distribution on the specimen makes the crack propagation path less dependent on the interface.

![Sampled CT scans of a ultra-high strength concrete](image1.png)

**Figure 7.2 Sampled CT scans of a ultra-high strength concrete**

<table>
<thead>
<tr>
<th>Sieve</th>
<th>AccumWt</th>
<th>% Passing</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. 4</td>
<td>0</td>
<td>100.00%</td>
</tr>
<tr>
<td>No. 8</td>
<td>0.3</td>
<td>99.94%</td>
</tr>
<tr>
<td>No. 16</td>
<td>8.6</td>
<td>98.35%</td>
</tr>
<tr>
<td>No. 30</td>
<td>19.9</td>
<td>96.19%</td>
</tr>
<tr>
<td>No. 50</td>
<td>162.5</td>
<td>68.91%</td>
</tr>
<tr>
<td>No. 100</td>
<td>245.2</td>
<td>53.09%</td>
</tr>
<tr>
<td>No. 200</td>
<td>291.3</td>
<td>44.27%</td>
</tr>
<tr>
<td>Pan</td>
<td>522.7</td>
<td>0.00%</td>
</tr>
</tbody>
</table>

**Table 7.1 Particle distribution analysis**

For the construction of the micro-geometry, a two-phase level set method is introduced for the image based void segmentation [136] as illustrated in Figure 7.3. The corresponding numerical discretization of the micro-geometry can then be obtained.

![Construction of numerical model through image segmentation](image2.png)

**Figure 7.3 Construction of numerical model through image segmentation**
7.2 Hierarchies of the Material Moduli

In this section, the numerical simulations for the different sizes of the RVE is performed to determine an appropriate RVE size. The homogenized material moduli obtained through the multi-scale modeling is adopted for the numerical simulations on the macroscopic level. A set of samples of the microscopic cells are chosen for numerical analyses to calculate the material moduli. As described in Chapter 6, if the micro-scale material moduli $C$ is an isotropic random field, $\tilde{C}^{RVE}$ should become an isotropic tensor [126] involving two Lamé constants $\tilde{\lambda}^{RVE}$ and $\tilde{\mu}^{RVE}$ (or the Young's modulus $\tilde{E}^{RVE}$ and shear modulus $\tilde{G}^{RVE}$) as the RVE size should be sufficiently large. Here the micro-scale material moduli are assumed to be isotropic, and consequently the homogenized material moduli $\tilde{C}^{RVE}$ is also isotropic. The homogenized material moduli $\tilde{E}^{RVE}$ and $\tilde{G}^{RVE}$ can then be easily determined through conducting uni-axial tensile and pure shear RVE analyses.

The material properties used in the microscopic level are Young's modulus $E=24.5$ MPa, and the Poisson's ratio $\nu=0.16$. A linear cohesive law with the tensile strength 3.48 MPa and fracture energy 1.0 N/m is employed. These parameters are curve fitted to the mean of the homogenized stress-strain curves and experimental data. Three different RVE sizes, 5x5 mm$^2$, 2.5x2.5 mm$^2$ and 1.25x1.25 mm$^2$, are used to identify the convergence of the material moduli. The smaller RVEs are obtained by equally partitioning each larger RVE into 4 sub-cells. Hence, the corresponding numbers of samples used are 500, 2000 and 8000 for the three different RVE sizes respectively. Three samples of different RVE sizes are shown in Figure 7.4 and Figure 7.5 displays the numerical results of the RVE analyses. The vertical coordinate of Figure 7.5 is the homogenized material moduli and the horizontal coordinate is the RVE size normalized by the largest void diameter of the micro-structure, which is 0.6 mm. Note here the equivalent Young's modulus obtained under the Dirchlete boundary condition is
normalized by a function of $\bar{v}_0$ as shown in (6.44), which is obtained from the largest microscopic cell. As can be seen in Figure 7.5, the ensemble averages of the material moduli converge to constants as the RVE size increases. The cases with the pure Dirichlet boundary condition and Neumann boundary condition serve as the upper bond and lower bond for the material moduli of SRVE, respectively. This matches the conclusion made in Chapter 6. For the case of the largest RVE size, the differences of the homogenized Young's modulus and the homogenized shear modulus between the upper and lower bonds are about 6.2% and 2.6%. The differences are normalized by the average of the homogenized material moduli of the largest RVE size under the Dirichlet boundary condition. Note that the limiting homogenized material moduli will eventually be located between the lower bond and upper bond. The values of the homogenized material moduli are chosen as the average of the upper bond and lower bond. Hence, the errors of the homogenized Young's modulus and the homogenized shear modulus for the largest RVE selected are 3.1% and 1.3%, respectively.

Figure 7.4 Samples of different microscopic cell sizes
The standard deviation (STD) of the homogenized material moduli normalized by the ensemble average is also computed as shown in Figure 7.6. The STD declines as the RVE size increases. As aforementioned in Chapter 6, the stochastic RVE approaches the deterministic RVE as the RVE size increases. Here the numerical results match the conclusion made in Chapter 6. However, the RVE size should also be sufficiently small compared with the structure size on the macroscopic level for the purpose of applying homogenization theory. Therefore, the material moduli still exhibit small uncertainties which need to be considered in the numerical analyses.

Figure 7.5 Convergence of the material moduli w. r. t. various RVE sizes

Figure 7.6 Standard deviation of the material moduli w. r. t. various RVE sizes
7.3 Tri-axial Compression Tests of the Ultra-high Strength Concrete with the Stochastic Multi-scale Modeling

Before conducting the numerical simulations on the macro-scale, the damage evolution functions used in the numerical tests should be determined. To evaluate the effects of the heterogeneity of the microstructure, the stochastic methods described in Chapters 3 and 4 are employed. A simple approach is to come up with an index that can quantitatively describe the structural behaviors. In this study, the factor which affects the microcrack propagation is void.

Two parameters are considered: the overall porosity and the maximum void size of each RVE sample. We define the porosity and the maximum void area of the microscopic cell to quantify the stochastic properties of voids in the micro-structure. The porosity is defined as:

\[
\text{Porosity} \equiv P = \frac{A_{\text{void}}}{A_{\text{cell}}} \quad (7.1)
\]

where \( A_{\text{void}} \) is the total area of the void and \( A_{\text{cell}} \) is the area of the microscopic cell. The porosity is considered as a random variable subjected to some assumed stochastic measures.

Figures 7.7(a) anb (b) show the probability density distribution of the porosity and the maximum void area normalized by the area of the RVE, which are obtained by using Kernel Density estimation (KDE) [137-138] with 1600 samples:

\[
\text{PDF}(x) = \frac{1}{N_{\text{sample}}} \sum_{j=1}^{N_{\text{sample}}} \frac{1}{\sqrt{2\pi h}} \exp \left[ -\frac{1}{2} \left( \frac{x - x_j}{h} \right)^2 \right] \quad (7.2)
\]

Where \( x \) is the concerned random variable. Here, \( x \) represents the porosity or the maximum void area of the microscopic cell. \( x_j \) is the porosity of the \( J \)-th sample, \( N_{\text{sample}} \) is the number of samples, and \( h \) is called the bandwidth of the kernel function. If the PDF of \( x \) is in a form close to Gaussian distribution, \( h \) is suggested as [139]
where $\sigma_x$ is the standard deviation of the random variable $x$. As illustrated in Figure 7.7(c), the Kernel Density Estimation is a graphical representation of the distribution of data which is closely related to histograms, but can be endowed with properties such as smoothness or continuity by using a suitable kernel.

As the PDFs of the porosity and the maximum void area is constructed, the Stochastic Collocation method described in Chapter 3 is introduced for the stochastic analysis. The collocation points are uniformly distributed in the random domain, which are the red points on the abscissa in Figure 7.7 (a) and Figure 7.7 (b). For each collocation point, the microscopic cell is selected from the sampling pool. These selected samples will be conducted using numerical simulations to obtain the corresponding damage evolution functions and then various damage laws will be applied on the macroscopic level to obtain the statistical quantities of the macrostructure.

$$h = \left(\frac{4}{3N_{\text{sample}}}\right)^{\frac{1}{2}}\sigma_x \tag{7.3}$$
On the microscopic level, the fracture mechanics based RVE analyses are conducted. The microscopic cell size of 5x5 mm$^2$ is chosen for the RVE analysis. This RVE with maximum cell dimension among the sampling pool corresponds to the minimum standard deviation in the homogenized moduli. The deviatoric and volumetric damage evolution functions are extracted by imposing pure Dirichlet shear and uni-axial tensile boundary conditions as described in Chapter 6. The material parameters in the RVE analysis are the same as those used in section 7.2. To determine which random variable, either the porosity $P$ or the normalized maximum void area $\hat{A}_{max}$ (normalized by the area of the RVE), has more influence on the material failure, the correlation coefficients $\rho_{f_u,P}$ and $\rho_{f_u,\hat{A}_{max}}$ are computed, where $f_u$ is the peak stress assumed to be a function of $P$, or $\hat{A}_{max}$, the correlation coefficients can be obtained by using the following formulas:

$$
\rho_{f_u,P} = \frac{E\left[(f_u - \mu_{f_u})(P - \mu_P)\right]}{\sigma_{f_u} \sigma_P}
$$

$$
\rho_{f_u,\hat{A}_{max}} = \frac{E\left[(f_u - \mu_{f_u})(\hat{A}_{max} - \mu_{\hat{A}_{max}})\right]}{\sigma_{f_u} \sigma_{\hat{A}_{max}}}
$$

where $E[\cdot]$ is the expectation operator, $\mu_{f_u}$, $\mu_P$, and $\mu_{\hat{A}_{max}}$ are the averages and $\sigma_{f_u}$, $\sigma_P$, and $\sigma_{\hat{A}_{max}}$ are the standard deviations of $f_u$, $P$ and $\hat{A}_{max}$, respectively. The correlation coefficients are computed based on the sampling data of RVE analyses, which are

$$
\rho_{f_u,P} = -0.38200, \quad \rho_{f_u,\hat{A}_{max}} = -0.08307, \quad \text{as } f_u = \text{Peak shear stress}
$$

$$
\rho_{f_u,P} = -0.37321, \quad \rho_{f_u,\hat{A}_{max}} = -0.07878, \quad \text{as } f_u = \text{Peak tensile stress}
$$

Note that $-1 \leq \rho_{x,y} \leq 1$. If a correlation coefficient $\rho_{x,y} = 0$, the two random variables $x$ and
y are uncorrelated. If $|\rho_{x,y}| = 1$, $x$ and $y$ are perfectly correlated. If $|\rho_{x,y}|$ is getting closer to 1, $x$ and $y$ are becoming more correlated. From (7.5), one can see that the porosity $P$ is much more correlated to the peak stress $f_u$ than $\hat{A}_{\text{max}}$, since $|\rho_{f_u,P}| > |\rho_{f_u,\hat{A}_{\text{max}}}|$ for both of the two loading cases. In this work, we consider a one-dimensional random space, hence the porosity is chosen as the sole random variable. The stress-strain curves and the damage evolution functions for the corresponding RVE analyses with different porosities are plotted in Figures 7.8 and 7.9. The failure patterns of a RVE sample under the tensile and shear loading cases are shown in Figure 7.10. The curves of the peak shear and tensile stresses vs. porosity are plotted in Figure 7.11. The regression curves describing the peak stresses are obtained by using the data from the RVE analyses by assuming they are second order polynomial functions:

$$f_u(P) = a_1 P^2 + a_2 P + a_3$$  \hspace{2cm} (7.6)

for $f_u = \text{Peak shear stress}$:

$$a_1 = 6.904 \times 10^7, \quad a_2 = 2.083 \times 10^6, \quad a_3 = 1.657 \times 10^6$$  \hspace{2cm} (7.7)

for $f_u = \text{Peak tensile stress}$:

$$a_1 = 2.058 \times 10^7, \quad a_2 = -2.594 \times 10^7, \quad a_3 = 5.678 \times 10^6$$

The statistical quantities of the porosity and peak stresses are:

$$\mu_p = 0.07055, \quad \sigma_p = 0.01306, \quad \frac{\sigma_p}{\mu_p} \times 100\% = 18.51\%$$  \hspace{2cm} (7.8)

Under shear loading:

$$\mu_{f_u} = 1.528 \text{ MPa}, \quad \sigma_{f_u} = 0.177 \text{ MPa}, \quad \frac{\sigma_{f_u}}{\mu_{f_u}} \times 100\% = 11.61\%$$  \hspace{2cm} (7.9)

Under uniaxial tension:

$$\mu_{f_u} = 4.354 \text{ MPa}, \quad \sigma_{f_u} = 0.646 \text{ MPa}, \quad \frac{\sigma_{f_u}}{\mu_{f_u}} \times 100\% = 14.83\%$$  \hspace{2cm} (7.10)

The normalized STDs of the homogenized material properties are listed in Table 7.2. The normalized standard deviation (STD) of the porosity is 18.51% while the normalized STDs of
the peak stresses are 11.61% and 14.83%, under the shear and tensile loading cases respectively. The normalized STDs of the peak stresses are slightly smaller than the one of the porosity, while for the Young's modulus and shear modulus, the normalized STDs are 3.4% and 4.6% respectively, which are much smaller than the normalized STD of the peak stresses. It's easy to realize why the peak stresses have much larger normalized STD. Since the peak stresses are determined after the cracks initiate and propagate, and the crack initiation is strongly affected by the void distribution in the microstructure, the crack paths become more unpredictable. Furthermore, the crack propagation is a continuous process and the deviations of the homogenized damage will be accumulated during the process. Hence, the overall material strength will exhibit larger uncertainty. On the other hand, the material moduli are determined at the elastic stage. No crack is formed at this stage. The determination of the material moduli is only related to the original configuration of the microstructure. The only factor affects the material moduli is the void distribution. Hence less STD of the material moduli are observed in the stochastic RVE analyses.

(a) Homogenized stress-strain curves  
(b) Damage evolution curves

Figure 7.8 RVE analyses under pure shear boundary condition
Figure 7.9 RVE analyses under uni-axial boundary condition

(a) Homogenized stress-strain curves  (b) Damage evolution curves

Figure 7.10 Failure patterns of an RVE sample under different loading conditions

(a) Under pure shear  (b) Under uniaxial tension

Figure 7.11 Peak stress-porosity curves

(a) Peak shear stress vs. porosity  (b) Peak shear stress vs. porosity
Table 7.2 Normalized STDs of the homogenized material properties

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Normalized STD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porosity</td>
<td>18.51%</td>
</tr>
<tr>
<td>Shear modulus</td>
<td>3.4%</td>
</tr>
<tr>
<td>Young’s modulus</td>
<td>4.6%</td>
</tr>
<tr>
<td>Peak shear stress</td>
<td>11.61%</td>
</tr>
<tr>
<td>Peak tensile stress</td>
<td>14.83%</td>
</tr>
</tbody>
</table>

On the macroscopic level, a set of experiments is considered to validate the proposed numerical models. Several cylindrical concrete specimens are tested under different confinement pressures. The dimension of the concrete cylinder used in the numerical simulation is 100 mm in diameter and 200 mm in height. Tests under different confinement stresses, namely, 20 MPa, 50 MPa, 100 MPa, and 300 MPa are adopted to compare the numerical results with the experimental data. Here the random variable $\xi$ employed in (6.126) is the normalized overall porosity of the RVE:

$$\xi = \frac{P - \mu_p}{STD_p}$$  \hspace{1cm} (7.11)

where $P$ is the overall porosity of the RVE, $\mu_p$ and $STD_p$ are the mean value and the standard deviation of $P$, respectively. In this case, the normalized standard deviation (STD) of the parameters $C_i^* \sim C_4^*$ and $\sigma_d^*$ are assumed to be the same as the normalized STD of the homogenized damage parameter $d^*$:

$$\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4 = \gamma = -\beta = -0.115$$ \hspace{1cm} (7.12)

where the normalized STD $|\beta|$ of $d^*$, which is the overall STD of the damage evolution, obtained from the multiscale modeling. The other parameters of the modified AFC model is listed in Table 7.3 which are characterized by the given triaxial experimental data.
Table 7.3 Parameters of the modified AFC model

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_1$</td>
<td>98.25 (MPa)</td>
</tr>
<tr>
<td>$C_2$</td>
<td>50 (MPa)</td>
</tr>
<tr>
<td>$C_3$</td>
<td>0.0125</td>
</tr>
<tr>
<td>$C_4$</td>
<td>0.002433</td>
</tr>
<tr>
<td>$A_n$</td>
<td>5.78x10^{-10} (1/Pa)</td>
</tr>
<tr>
<td>$h_a$</td>
<td>13</td>
</tr>
<tr>
<td>$h_b$</td>
<td>0.5</td>
</tr>
<tr>
<td>$a_1$</td>
<td>0.3747x10^8</td>
</tr>
<tr>
<td>$a_2$</td>
<td>-0.1985</td>
</tr>
<tr>
<td>$a_3$</td>
<td>-0.0049x10^{-8}</td>
</tr>
</tbody>
</table>

Note: $a_1, a_2$ and $a_3$, are the parameters used in (6.125)

The Young's and shear moduli obtained through the microscopic cell analyses as aforementioned in section 7.2, can be expressed as

\[
E' = \langle \bar{E} \rangle (1 - k_1 \xi), \quad k_1 = 0.034, \\
G' = \langle \bar{G} \rangle (1 - k_2 \xi), \quad k_2 = 0.046
\]  

(7.13)

where $\langle \bar{E} \rangle$ and $\langle \bar{G} \rangle$ are the means of the effective Young's modulus and shear modulus and the $k_1$ and $k_2$ are the normalized STD as shown in Figure 7.6.

The RK approximation discussed in Chapter 4 is introduced in the probability domain to re-interpolate the stress field in terms of the random variable, which is the porosity of the RVE. The corresponding statistical stress-strain curves are obtained by using the RK approximation with the corresponding PDF. More specifically, the major principle stress of the concrete specimens can be expressed in terms of the axial strain $\varepsilon$ and the random variable $\xi$, which is the porosity of the RVE:

\[
\sigma_p = \sigma_p(\varepsilon, \xi)
\]  

(7.14)

There are 11 samples $\xi = \xi_1, \cdots, \xi_{11}$ in the random domain. Therefore the stress strain relationships in respond to the samples can be obtained by conducting RVE analyses:
\[ \sigma_{\rho_i} = \sigma_{\rho}(\varepsilon, \xi_i), \]
\[ \vdots \]
\[ \sigma_{\rho_{11}} = \sigma_{\rho}(\varepsilon, \xi_{11}) \]  

Introduce the RK approximation in the random domain:

\[ \sigma_{\rho}(\varepsilon, \xi) = \sum_{I=1}^{NP} \Psi_I(\xi) \hat{\sigma}_I(\varepsilon) \]  

The coefficients \( \hat{\sigma}_I(\varepsilon) \) at some \( \varepsilon \) are then solved by substituting the solution of each collocation point into the above equation:

\[ \sigma_{\rho}(\varepsilon, \xi_i) = \sum_{I=1}^{NP} \Psi_I(\xi_i) \hat{\sigma}_I(\varepsilon) \]
\[ \vdots \]
\[ \sigma_{\rho}(\varepsilon, \xi_{11}) = \sum_{I=1}^{NP} \Psi_I(\xi_{11}) \hat{\sigma}_I(\varepsilon) \]  

Here, 11 source points are used for the RK approximation. The coefficients are then obtained by using least square method as shown in (3.58). For estimation of the statistical moments, such as mean and standard deviation, the following equations are employed:

\[ \mu_{\sigma_{\rho}(\varepsilon)} = \int_{\Omega} \rho(\xi) \sum_{I=1}^{NP} \Psi_I(\xi) \hat{\sigma}_I(\varepsilon) d\xi \]  

\[ STD_{\sigma_{\rho}(\varepsilon)} = \sqrt{\int_{\Omega} \rho(\xi) \left( \sum_{I=1}^{NP} \Psi_I(\xi) \hat{\sigma}_I(\varepsilon) - \mu_{\sigma_{\rho}(\varepsilon)} \right)^2 d\xi} \]  

where \( \mu_{\sigma_{\rho}(\varepsilon)} \) and \( STD_{\sigma_{\rho}(\varepsilon)} \) are the mean and the standard deviation of the major principle stress at some value of axial strain \( \varepsilon \) and \( \rho(\xi) \) is the probability density function of the porosity as shown in 7.7 (a).

As discussed in Chapter 6, as the RVE size is inconsistent with the mesh size, the numerical results exhibit mesh dependency. To remedy the mesh dependency, a discretization with mesh size close to the RVE size is adopted to simulate the problem. The comparisons between the numerical simulations and the experiments are plotted in Figure 7.12. For the
numerical simulations, three curves are obtained through the stochastic analysis for each confinement stress. One is the average of the principal stress difference, which is the difference between the major principal stress and the confinement stress, and the other two are the average ± STD.

![Graphs showing tri-axial compression tests](image)

(a) 20 MPa confinement stress  
(b) 40 MPa confinement stress  
(c) 100 MPa confinement stress  
(d) 300 MPa confinement stress

**Figure 7.12 Comparison of the tri-axial compression tests**

In the comparison, the numerical results appropriately agree with the experimental data. Note that as high confinement stresses, such as 100 MPa and 300 MPa, the material still exhibits strong stiffness after reaches the yield point. The stiffness is appropriately captured by the additional hardening law in the AFC model. As the load reaches the limit point, where the material hardening stiffness is dropped and the damage started to evolve, the yield strength stops increasing and slightly decreasing until the strain reaches the unloading point.

For the case with low confinement stress, the numerical model does not perfectly capture the initial yield point. In the experiments, the initial yield strength is in the range from about 80 MPa to 150 MPa, which did not notably grow with the increased confinement, and for some
cases, e.g. confinements of 20 MPa and 50 MPa, the initial yield strength is even slightly dropped. The decline of the initial yield strength with increased confinement is difficult to be captured by the AFC model, where the yield surface grows with the increasing pressure. Due to the complexity of the material under consideration, the ACF model appears to be adequate only within a finite range of the confinement.
CHAPTER 8

Conclusions and Future Work

This dissertation aims to develop a multi-scale stochastic damage model for brittle materials. The material failure observed on the macro-scale has been considered as the consequence of the crack formation and coalescence in the micro-scale. Due to the need for micro-crack informed stochastic multi-scale modeling for the construction of stochastic damage model, several numerical approaches have been proposed for the stochastic analyses. Developments of crack modeling and multi-scale damage modeling have also been carried out in this work. Further, several methods have been proposed to enhance the accuracy of the numerical modeling of the concerned problems.

8.1 Summary of Developments

The conventional generalized polynomial chaos (gPC) method employs orthogonal bases with respect to the probability density function for the approximation of random variables. This leads to considerable errors in problems where the regularity of the probability density function is not consistent with gPC. In this work, the RBF and RK approximations have been introduced to represent the stochastic variables. In conjunction with the stochastic collocation methods, the proposed algorithm has been shown to enhance the accuracy and convergence of the polynomial chaos approach. Furthermore, the proposed collocation method allows the stochastic differential equation to be solved with a series of deterministic systems, which is
suitable for parallel computation. Since the approximation in the random domain can be defined as a tensor product, the RK approximation with equally spaced discretization and virtual points outside the boundaries degenerates to periodic functions. This approach significantly reduces computational complexity without sacrificing accuracy or rate of convergence. On the other hand, the construction of directional transformation matrices and the use of the decomposed Gaussian elimination for problems of high dimensionality which have a random domain significantly reduces the computational expense while not affecting the accuracy of the approximation.

For the fracture problem, an extrinsically enriched RKPM has been introduced to model the crack propagation. A new enrichment scheme has been proposed which utilizes the visibility criterion while preserving the Partition of Unity (POU) property for the enriched mesh-free approximation function, which guarantees the mass conservation of the discrete system. Consequently, the explicit time integration is employed for the crack propagation modeling. The proposed enrichment method has been verified by conducting several benchmark fracture problems. Furthermore, since the RK shape functions are rational and the near-tip enrichment functions are either singular in LEFM or highly nonlinear when cohesive zone model or the visibility criteria are adopted, the conventional Gauss quadrature cannot guarantee to meet integration constraint. As a result, the Galerkin approximation loses the Galerkin orthogonality [107] and the loss of optimal convergence in the solution. A method for domain integration has been proposed for Galerkin approximation. The scheme for domain integration is designed to satisfy an arbitrary order integration constraint which was addressed by Chen et al. [105-106] and Rüter et al. [107] to restore the Galerkin orthogonality. The accuracy of the solution, especially for the near-tip fields, has been improved by enforcing variational consistency of the Galerkin formulation. The
computational cost for domain integration has also been significantly reduced as demonstrated in the numerical examples.

For the stochastic multi-scale modeling, this work is the extension of the micro-crack informed damage model by Ren and Chen et al. [82]. In addition to this approach, stochastic variations of the micro-geometry have been considered in this dissertation. The characteristics of the stochastic representative volume element (SRVE) have been investigated. The existence of SRVE has been confirmed through the satisfaction of the Hill condition, ergodicity and the principle of the minimum potential energy, where the first two are assumptions and the last one is due to the nature of the continuum mechanics. As a sufficient RVE size is used such that the averaged material quantities converge, the existence of RVE has been demonstrated. The size effect of the damage modeling is also demonstrated by using the principle of the minimum potential energy, which asserts that a structure or body shall deform or displace to a position as in equilibrium that minimizes the total potential energy. Any perturbation from the equilibrium situation of a structure will only cause the increase of the potential energy. Moreover, the issue of the mesh dependency is then further addressed. To resolve the mesh dependency, a damage evolution with a size scaling law is proposed to obtain mesh insensitive results.

Finally, a two-parameter multi-scale damage model has been proposed under the framework of the SRVE, which considers the shear and volumetric failure for brittle materials. The yield criterion of the proposed model follows the Advanced Fundamental Concrete (AFC) model, while the damage evolution is obtained from the multi-scale energy bridging method. The proposed multi-scale damage model was then validated through the comparisons between the numerical and the experimental results of the concrete materials under tri-axial
8.2 Suggestions for Future Work

(1) *Further development of the generalized stochastic chaos*

In the current work, the generalized stochastic chaos and the corresponding numerical algorithms have been proposed to enhance the accuracy and efficiency of the commonly used stochastic polynomial chaos. However, for a large and complicated stochastic system, the computational cost is still high. An adaptive stochastic method based on the proposed generalized stochastic chaos is suggested to further enhance the computational efficiency for large systems with desired accuracy.

(2) *Development of the multi-phase micro-scale modeling*

A multi-phase model of concrete material can be considered next. Typically, concrete material is composed of voids, aggregates, matrix and the interface. If the aggregates are much stronger than the matrix, or the bonding strength of the interface is much weaker than the two materials, the initiation and growth of micro-cracks will be strongly affected by the layout of the micro-structure. This may result in a different failure mechanism or change the characteristics of stochastic behaviors from the simplified two-phase model.

(3) *Consideration of the fiber-reinforced concrete*

Fiber-reinforced concrete can be considered in the future. Fibers are usually used in concrete to control cracking due to plastic and drying shrinkage. Consequently, material tensile strength can be improved through fiber reinforcement. For the fracture-mechanics based RVE analyses, the cohesive model may be a good candidate to evaluate the effects of fibers on the growth of micro-cracks and how the failure behaviors of the concrete...
material are affected by the fiber reinforcement. The reinforcement of the fibers can be modeled as cohesive tractions on the crack surfaces with appropriate cohesive laws.
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158